



Draft Toxic Weighting Factor Development in Support of CWA 304(m) Planning Process

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SECTION 1

INTRODUCTION

1.1 INTRODUCTION

In 1981, EPA's Office of Water convened a Cost-Effectiveness (C-E) Task Force. Once developed, the Task Force's methodology (called C-E methodology) has been applied to all subsequent rulemaking efforts and has basically withstood the test of time, Office of Management and Budget (OMB) review, and the courts (Ehrensberger and Rico, 1988). All cost-effectiveness calculations are deflated to 1981 dollars—the year of the Task Force. The Task Force selected the Engineering News Record Construction Cost Index (CCI) as the index to be used when deflating the costs to 1981 dollars.

C-E methodology is an approach to evaluating a series of pollution control technology trains within an industry, subcategory, or segment of an industry. In particular, C-E compares the incremental costs of moving from one technology train option to another with the incremental removals associated with that change. The procedure identifies “inefficient” options that cost more but remove less pollutants. When the options are ranked by increasing pollutant removals and plotted against cost, the investigator can visually identify the “elbow in the curve,” where it becomes much more expensive to remove fewer additional pollutants.

Because each pollutant has its own level of toxicity, it was necessary to develop toxic weighting factors (TWFs). Without such a factor, a pound of tetrachloro-dibenzo-*p*-dioxin, 2,3,7,8 would have the same “value” (in terms of removal) as a pound of copper. TWFs were developed to be protective of both human and aquatic life. Section 2 summarizes the TWF methodology.

By converting chemical discharges to a “toxic-weighted pounds-equivalent” basis, TWFs provide a mechanism by which discharges containing different mixtures of chemicals can be compared. For effluent guideline development, the comparison is the relative efficiency of different technology train options in removing chemicals within a given industry or industry segment. The comparison is the C-E methodology described in the paragraph above. For planning purposes, such as the 304(m) process, the discharges from different industries can be compared on a toxic-weighted pounds-equivalent basis

(TWPE) to identify industries, subcategories, or segments of an industry for which additional pollution controls might be beneficial.

The initial list of pollutants considered in a C-E analysis focused on priority pollutants.¹ As effluent limitations guidelines were developed for more and more industries, the number of pollutants for which EPA developed TWFs also increased. At present, EPA has developed TWFs for approximately 1,900 chemicals.

The C-E methodology was originally intended as a “within-an-industry” analytical tool to evaluate different technology train options. EPA routinely reviewed and updated TWF data at various points in the rulemaking schedule (e.g., option selection), but at any given point in time, all pollutants within an industry were compared with the same set of TWFs. EPA might not have had cause to update a pollutant that was detected in wastewater discharges from an industry regulated in the early 1980s if it was not detected in wastewater discharges from industries regulated after that time.

Section 304(b) of the Clean Water Act requires EPA to review effluent guidelines for existing direct dischargers each year and to revise the regulations as appropriate. Section 304(b) also specifies factors that EPA must consider when deciding whether to revise an effluent guideline. Section 304(m) supplements the core requirement of Section 304(b) by requiring EPA to publish a plan every two years announcing its schedule for this annual review, as well as its schedule for any guideline revision that results from the review. EPA has published a final Plan under Section 304(m), every even-numbered year since 1990, that describes these activities. For the 2004 Plan, EPA developed and proposed a draft Strategy for National Clean Water Industrial Regulations (“National Strategy”) (EPA, 2002) to outline how EPA would address the factors outlined in Section 304(b). The first factor in the strategy considers the amount and toxicity of the pollutants remaining in an industrial category’s discharge. TWFs were used with discharges reported in the Toxics Release Inventory (TRI) and the Permit Compliance System (PCS) to generate preliminary rankings by industry (EPA, 2004).

With the National Strategy, TWFs underwent a change in role and were used in “industry-to-industry” comparisons. Accordingly EPA decided to develop a TWF database that serves as a self-

¹These pollutants are discussed in the Clean Water Act (33 USC 1317) Section 307a and Code of Federal Regulations, Title 40, Part 423, Appendix A.

contained reference for TWF development. The initial version of the database is the source of the “August 2004” TWF values. EPA developed a list of updates and revisions (Zipf, 2003) that it then incorporated in the database. After revisions and updates, the set of about 1,900 TWFs was called the “December 2004” TWF values.

Section 2 presents EPA’s methodology for developing TWFs as well as the revisions and updates to the August 2004 values. Section 3 presents the TWF development for the special case of dioxin and its congeners. The database is described briefly in Section 4 while Section 5 compares the August and December values. As EPA’s development of effluent limitations guidelines continues, there is an ongoing need for TWFs for new pollutants or groups of pollutants. Ongoing efforts are summarized in Section 6.

1.2 REFERENCES

Ehrensberger, K., and R. Rico. 1988. Cost-effectiveness analysis for effluent guidelines. United States Environmental Protection Agency, Office of Water Regulations and Standards, Economic Analysis Branch. May.

EPA. 2004. Notice of availability of 2004 effluent guidelines program plan. Fed. Reg. 69:53,705–53,721. September 2.

EPA. 2002. Draft strategy for national clean water industrial regulations. Fed. Reg. 67:71,665–71,169. November 29.

Zipf, L. 2003. Revisions to EAD’s toxic weighting factor methodology parameters. Memorandum to 304(m) record (EPA docket number OW-2003-0074). December 3.

SECTION 2

CURRENT METHODOLOGY

This section provides a brief overview of the methodology for calculating TWFs and is drawn from Zipf (2003). The methodology was first established in 1981 by EPA's Cost-Effectiveness Task Force. One modification to the methodology occurred when the water quality criterion for copper was updated in 1985 (Ehrensberger and Rico, 1988). This is noted in the text below.

The discussion works backward from the TWF (Section 2.1) into its component human health and aquatic health components. Sections 2.2 and 2.3 provide additional information for the human and aquatic health values, respectively, including the preference order for data sources. All effluent guidelines promulgated under the 1992 Consent Decree used the methodology described in this section in the C-E analyses. These values are discussed in the Development Document as the "August 2004" TWF values (EPA, 2005a). During the latter part of 2004, EPA incorporated updates and revisions to the methodology and basic data values; these are the "December 2004" TWF values.

2.1 ADDITION OF HUMAN AND AQUATIC HEALTH VALUES

TWFs are derived from chronic aquatic life criteria (or toxic effect levels) and human health criteria or toxic effect levels established for the consumption of fish. For carcinogenic substances, EPA sets the human health risk level at 10^{-5} (i.e., protective to a level allowing 1 in 100,000 excess lifetime cancer cases over background). In the TWF method for assessing water-based effects, these toxicity levels of pollutants of concern are compared to a benchmark value that represents the toxicity level of a specified pollutant. EPA selected copper, a toxic metal commonly detected and removed from industrial effluent, as the benchmark pollutant. EPA had used copper in previous TWF calculations for the cost-effectiveness analysis of effluent guidelines; although EPA revised the water quality criterion for copper in 1998 (to 9.0 micrograms per liter, or $\mu\text{g/L}$), the TWF method uses the former criterion ($5.6 \mu\text{g/L}$) to facilitate comparisons with cost-effectiveness values calculated for other regulations. This was considered valid because all CE measures are relative (Ehrensberger and Rico, 1988). The former criterion for copper ($5.6 \mu\text{g/L}$) was reported in the 1980 *Ambient Water Quality Criteria for Copper* document (EPA, 1980).

To calculate TWF values, EPA adds TWFs for aquatic life effects and human health effects for each pollutant of concern. EPA uses chronic effects on aquatic life and human health effects from ingesting contaminated organisms (HHOO) as the basis for TWFs. To make the calculation, EPA divides aquatic life and human health criteria (or toxic effect levels) for each pollutant, expressed as a concentration in µg/L, into the former copper criterion of 5.6 µg/L:

$$\text{TWF} = \frac{5.6}{\text{AQ}} + \frac{5.6}{\text{HHOO}}$$

where:

TWF = toxic weighting factor

AQ = chronic aquatic life value (µg/L)

HHOO = human health value (organisms only) (µg/L)

2.2 HUMAN HEALTH CRITERIA

EPA calculates the human health component of a TWF based on consumption of contaminated organisms. Therefore, EPA envisioned a scenario in which a person would fish or harvest shellfish for consumption. The water body in this scenario would not necessarily be a drinking water source. Even if it were, EPA reasoned, treatment at the drinking water plant would address any contamination.

2.2.1 Effects and Risk Levels

As stated in Section 2.4 of the 2000 Methodology for Deriving Ambient Water Quality Criteria for the Protection of Human Health, “EPA believes that both 10^{-6} and 10^{-5} may be acceptable for the general population....adoption of a 10^{-6} or 10^{-5} risk level...represents a generally acceptable risk management decision” (EPA, 2000).

For chemicals that (1) have both a reference dose (RfD) value for non-carcinogenic effects and a slope factor (SF) value for carcinogenic effects and (2) draw those RfD and SF values from sources in the same level of the hierarchy (see below), the human health values are calculated using the SF, which is always the more stringent value of the two. When a chemical has both an RfD and SF but these values are from different levels of the hierarchy, the value from the source higher on the hierarchy is used.

2.2.2 Hierarchy of Data Sources

EPA follows a hierarchy of data sources to determine human health values. This hierarchy is based on Section 2.4.6 of the *Technical Support Document for Water Quality-Based Toxics Control* (EPA, 1991), which recommends using the most current risk information from EPA's Integrated Risk Information System (IRIS) when estimating human health risks. The hierarchy is:

- Calculated human health criteria using IRIS (EPA, 2005b) oral RfDs or oral cancer potency SFs in conjunction with adjusted 3 percent lipid bioconcentration factor (BCF) values derived from *Ambient Water Quality Criteria Documents* published during the 1980s (EPA, 2005c). Three percent is the mean lipid content of fish tissue reported in the study from which the average daily fish consumption rate of 6.5 grams per day (g/day) was derived (EPA, 1991).
- Calculated human health values using current IRIS RfDs or SFs and representative unadjusted BCF values for common North American species of fish or invertebrates or estimated BCF values.
- Calculated human health values using RfDs or SFs from EPA's Health Effects Assessment Summary Tables (HEAST) or EPA's Region III Risk-Based Concentration (RBC) Table (EPA, 2004) used in conjunction with adjusted 3 percent lipid BCF values derived from *Ambient Water Quality Criteria Documents*.
- Calculated human health criteria using current RfDs or SFs from HEAST or EPA's Region III RBC table and representative BCF values for common North American species of fish or invertebrates or estimated BCF values.
- Criteria from the *Ambient Water Quality Criteria Documents*.
- Calculated human health values using RfDs or SFs from data sources other than IRIS, HEAST, or the Region III RBC Table.

2.2.3 Deriving Ambient Water Quality Criteria for the Protection of Human Health—1980 Methodology and 2000 Revisions

In 2000, EPA published revisions to its "2000 methodology" for deriving ambient water quality criteria for the protection of human health (EPA, 2000a and 2000b). Zipf (2003) identified the need to update the TWF calculations to reflect these revisions:

- Change average daily fish consumption rate from 6.5 grams to 17.5 grams/day to adequately protect the general population of fish consumers.
- Change from bioconcentration factors (BCFs) to bioaccumulation factors (BAFs). Section 2.2.3.1 discusses how this change is incorporated into the model.
- Incorporate a relative source contribution (RSC) to account for non-water sources of exposure. Section 2.2.3.2 discusses how this change is incorporated into the model.

Tables 2-1 and 2-2 present the equations for calculating human health criteria with both the 1980 and 2000 methodologies. The equation accounts for effect (cancer or non-cancer) and pathway (organism only or water and organism).

The August 2004 TWF database is based on the 1980 methodology. The December 2004 TWF database is based on the 2000 methodology and subsequent water quality criteria updates for specific chemicals (see Section 2.2.4 below).

Table 2-1

Comparison of 1980 and 2000 Methodologies for Calculating Human Health Criteria Based on Slope Factors

1980 Methodology	2000 Methodology
Carcinogenicity Protection	
<p>Ingestion of Organisms Only</p> $\text{HHOO (ug / L)} = \frac{\left(\text{Risk level}(10^{-5}) / q1^* \right) \times 70 \text{ kg} \times 1,000 \text{ ug / mg}}{0.0065 \text{ kg / day} \times \text{BCF(L / kg)}}$	<p>Ingestion of Organisms Only</p> $\text{HHOO (ug / L)} = \frac{\left(\text{Risk level}(10^{-5}) / q1^* \right) \times 70 \text{ kg} \times 1,000 \text{ ug / mg}}{0.0175 \text{ kg / day} \times (\text{BCF(L / kg)} \text{ or } \text{BAF(L / kg)})}$
<p>Ingestion of Water and Organisms</p> $\text{HHWO (ug / L)} = \frac{\text{Risk level}(10^{-5}) \times 70 \text{ kg} \times 1,000 \text{ ug / mg}}{q1^* (\text{mg / kg - day}) \times [2 \text{ L / day} + [0.0065 \text{ kg / day} \times \text{BCF(L / kg)}]]}$	<p>Ingestion of Water and Organisms</p> $\text{HHWO (ug / L)} = \frac{\left(\text{Risk level}(10^{-5}) / q1^* \right) \times 70 \text{ kg} \times 1,000 \text{ ug / mg}}{[2 \text{ L / day} + [0.0175 \text{ kg / day} \times (\text{BCF(L / kg)} \text{ or } \text{BAF(L / kg)})]]}$

where:

70 kg = body weight
 2 L/day = daily drinking water intake
 0.0065 kg/day = daily fish intake (1980)
 0.0175 kg/day = daily fish intake (2000)
 RfD = reference dose
 q1* = cancer potency factor or cancer slope factor
 RSC = relative source contribution
 BAF = bioaccumulation factor
 BCF = bioconcentration factor

Table 2-2

Comparison of 1980 and 2000 Methodologies for Calculating Human Health Criteria Based on Reference Doses

1980 Methodology	2000 Methodology
Toxicity Protection	
<p>Ingestion of Organisms Only</p> $\text{HHOO (ug / L)} = \frac{\text{RfD (mg / kg / day)} \times 70 \text{ kg} \times 1,000 \text{ ug / mg}}{0.0065 \text{ kg / day} \times \text{BCF(L / kg)}}$	<p>Ingestion of Organisms Only</p> $\text{HHOO (ug / L)} = \frac{\text{RfD (mg / kg / day)} \times \text{RSC} \times 70 \text{ kg} \times 1,000 \text{ ug / mg}}{0.0175 \text{ kg / day} \times (\text{BCF(L / kg)} \text{ or } \text{BAF(L / kg)})}$
<p>Ingestion of Water and Organisms</p> $\text{HHWO (ug / L)} = \frac{\text{RfD (mg / kg / day)} \times 70 \text{ kg} \times 1,000 \text{ ug / mg}}{2\text{L / day} + [0.0065 \text{ kg / day} \times \text{BCF(L / kg)}]}$	<p>Ingestion of Water and Organisms</p> $\text{HHWO (ug / L)} = \frac{\text{RfD (mg / kg / day)} \times 70 \text{ kg} \times 1,000 \text{ ug / mg}}{2\text{L / day} + [0.0175 \text{ kg / day} \times [\text{BCF(L / kg)} \text{ or } \text{BAF(L / kg)}]]}$

where:

70 kg	=	body weight
2 L/day	=	daily drinking water intake
0.0065 kg/day	=	daily fish intake (1980)
0.0175 kg/day	=	daily fish intake (2000)
RfD	=	reference dose
q1*	=	cancer potency factor or cancer slope factor
RSC	=	relative source contribution
BAF	=	bioaccumulation factor
BCF	=	bioconcentration factor

2.2.3.1 BCFs and BAFs

Bioconcentration is the uptake and retention of a chemical by an aquatic organism from water only. Bioaccumulation is the uptake and retention of a chemical from all surrounding media (e.g., water, food, and sediment). For some chemicals, e.g., those that are highly persistent and hydrophobic, bioaccumulation can be far larger than bioconcentration. EPA (2000a) recommends shifting from BCFs to BAFs in the calculation of water quality criteria for human health.

EPA 2000a outlines separate procedures for deriving national BAFs depending on the type of chemical, such as nonionic organic, ionic organic, inorganic, and organometallic. It also recommends the use of a weighted-average BAF that incorporates four trophic levels, e.g.:

$$\text{BAF} = \sum_{i=2}^4 \text{FI}_i \times \text{BAF}_i$$

where:

FI_i = fish intake at trophic level I where I = 2, 3, and 4

BAF_i = bioaccumulation factor at trophic level I where I = 2, 3, and 4

The time- and resource-intensive nature of estimating national BAFs is cited as the reason why EPA did not include BAFs in the human health criteria in the National Recommended Water Quality Criteria: 2002 (EPA 2002a). To keep the TWF model as flexible as possible, it is structured to use a BAF value if one exists and a BCF value if one does not.

2.2.3.2 Relative Source Contribution Factors

The TWF model is structured to calculate a human health criterion based on the 2000 methodology including an RSC factor. The model is populated with the RSC values where they are reported in the *National Recommended Water Quality Criteria: 2002* (EPA, 2002a) and in Bell (2000).² The values reported by Bell are listed in Table 2-3.

²The default value for an RSC is 1.

2.2.4 Water Quality Criteria Updates Since 2000

EPA updated the TWF models with the data presented in *National Recommended Water Quality Criteria: 2002* (EPA, 2002a). The values for the components for calculating human health criteria were taken from the support document (EPA, 2002b). For some chemicals, however, EPA (2002a) continues to calculate water quality criteria based on the 1980 methodology. The TWF model is programed to select the human health component as calculated by the 2000 methodology for organism only ingestion. A separate variable was added to the model to flag when the TWF should use the 1980 methodology for calculating the human health component. This was done in order to make the TWF model consistent with EPA (2002a) unless superceded by a later EPA publication.

On the last day of 2003, EPA published updated national water quality criteria for human health for 15 chemicals (EPA, 2003a).³ EPA incorporated the updated RfD, q1*, RSC, and BCFs into the TWF database for the December 2004 version.

³Chlorobenzene; cyanide; dichlorobenzene, 1,2; dichlorobenzene, 1,4; dichloroethylene, 1,1; dichloropropene, 1,3; endrin; ethylbenzene; hexachlorocyclopentadiene; lindane; thallium; toluene; transdichloroethylene, 1,2; trichlorobenzene, 1,2,4; and vinyl chloride.

Table 2-3
Uncertainty Factors and Relative Source Contributions

Chemical	Uncertainty Factors		RSC (%)
	Regular	Carcinogenic	
antimony	1000	—	40
atrazine	100	10	20
barium	3	—	NA
beryllium	100	10	20
cadmium	10	—	25
carbofuran	100	—	20
chromium	100	—	71
chlorobenzene	1000	—	20
copper	2	—	NA
cyanide	100	—	20
2,4-D	100	—	20
dalapon	100	—	20
p-dichlorobenzene	1000	10	20
o-dichlorobenzene	1000	10	20
di(2-ethylhexyl) adipate	100	10	20
1,1-dichloroethylene	1000	10	20
cis-1,2-dichloroethylene	3000	—	20
trans-1,2-dichloroethylene	1000	—	20
dinoseb	1000	—	20
diquat	100	—	20
endrin	100	—	20
ethylbenzene	1000	—	20
endothall	100	—	20
glyphosate	100	—	20
hexachlorocyclopentadiene	1000	—	20
lindane	1000	10	20
methoxychlor	1000	—	20
mercury	1000	—	20
oxamyl	100	—	20
picloram	100	—	20

Table 2-3
Uncertainty Factors and Relative Source Contributions

Chemical	Uncertainty Factors		RSC (%)
	Regular	Carcinogenic	
simazine	1000	10	20
styrene	1000	10	20
2,4,5-TP	100	—	20
thallium	1000	—	20
toluene	1000	—	20
1,2,4-trichlorobenzene	1000	—	20
1,1,2-trichloroethane	1000	10	20
1,1,1-trichloroethane	1000	—	20
xylenes	100	—	20

NA: not appropriate, usually for uncertainty factors and/or RSCs with respect to maximum contaminant level goals and lifetime health averages set on the basis of human data, not animal research data.

Source: Bell, 2000.

2.3 CHRONIC AQUATIC LIFE VALUES

When selecting chronic aquatic toxicity values, EPA uses national water quality criteria, when available. When these criteria are not available, other values representative of the chemical's chronic toxicity are used. Sections 2.3.1 through 2.3.4 list various data sources for aquatic life values in the same order as those sources appear in EPA's hierarchy.

2.3.1 National Chronic Freshwater Quality Criteria

National chronic water quality criteria are the first choice for values because they represent a consideration of a chemical's toxicity to wide range of aquatic life and have been published by EPA. The EPA Office of Water describes the derivation of criteria values in documents for specific pollutants (EPA, 2005c). A national chronic water quality criterion is defined as the 4-day average concentration of a toxicant at which a wide range of aquatic organisms should not be unacceptably affected, provided that average is not exceeded more than once every 3 years.

2.3.2 Lowest Reported Measured Maximum Allowable Toxicant Concentration, Lowest-Observed-Effect Concentration, or No-Observed-Effect Concentration

The term “chronic” refers to a stimulus that continues over time, often for periods of several weeks to years, depending on the affected organism’s reproductive life cycle. The biological response to the exposure typically progresses slowly and lasts a long time. Chronic aquatic tests measure the effects of long-term exposure to a chemical; citing rapid developments in test methodology, EPA recommends several 7-day, short-exposure-duration test methods (EPA, 1989). Test endpoints include such variables as survival percentage, hatchability, and normal larva weight and length. Chronic tests of longer exposure duration measure endpoints such as growth and reproduction.

EPA uses chronic aquatic test data to identify three concentration levels of potential significance: the no-observed-effect concentration (NOEC), the lowest-observed-effect concentration (LOEC), and the maximum allowable toxicant concentration (MATC). The NOEC—the highest toxicant concentration to which test organisms have been exposed with no observed adverse effects—can be statistically determined using hypothesis testing or derived from the inhibition concentration. This inhibition concentration is an estimate of the toxicant concentration that will cause a given percentage reduction in biological measurement of the test organisms. The LOEC is the lowest toxicant concentration at which a chronic effect on a test organism has been observed. The MATC is the geometric mean of the NOEC and LOEC and is meant to represent the threshold level where chronic effects will begin to occur. MATC values are selected first, followed by LOEC values and then NOEC values for use in calculating TWFs.

2.3.3 Lowest Chronic or Reproductive Test Concentration

For chemicals that do not have chronic aquatic life criteria, MATCs, LOECs, or NOECs, EPA obtains chronic effect concentrations from readily available sources of chronic toxicity test data. The preferred information source is EPA’s Assessment Tools for the Evaluation of Risk (ASTER), which combines the Aquatic Toxicity Information Retrieval database (AQUIRE), the EPA Environmental Research Laboratory–Duluth (ERL-Duluth) fathead minnow database, and tables of toxicity test results from water quality criteria documents (EPA, 2005d).⁴ The ASTER system differentiates between

⁴Access to ASTER is restricted as of January 2004 (see http://www.epa.gov/med/Prods_Pubs/aster.htm, downloaded September 15, 2004). ASTER technical

AQUIRE test data that are likely to be of good quality and AQUIRE test data that are of unknown quality, according to the following criteria:

- Test pH within the range of 6.5 to 8.5.
- Review code 1 (methodology section cites published or well-documented procedures; satisfactory control; measured concentration; temperature, pH, dissolved oxygen, and hardness are reported) or code 2 (one or more of the following may occur: control mortality not reported; no solvent control when a solvent is used in the test; unmeasured concentration; water chemistry variables not reported or incomplete).
- No use of formulations or carriers.
- Measured values and flow-through exposure only for tests on fish (no static exposure).
- Measured values only for invertebrates or plants (exposure may be static or flow-through).

Test results from the ERL-Duluth fathead minnow database are assumed to be of good quality. However, test results reported in water quality criteria documents are assumed to be of unknown quality.

EPA selects the lowest reported concentration—from a chronic growth or reproductive test on a North American native fish or invertebrate or from a biologically significant EC₅₀ test for an algal species (e.g., chlorophyll production)—from the pool of test data likely to be of good quality or, alternatively, from the pool of data of unknown quality. If appropriate test data are not available from ASTER, other primary or secondary information sources are consulted.

2.3.4 Estimated Chronic Toxicity Concentration from a Measured Acute: Chronic Ratio for a Less Sensitive Species, Quantitative Structure-Activity Relationship Model, or Default Acute: Chronic Ratio of 10:1

EPA uses estimated chronic toxicity concentrations when measured values are unavailable. The first option for estimating a chronic toxicity concentration is to use acute toxicity concentrations and a measured acute:chronic ratio (ACR). ACRs are based on measured acute and chronic pollutant concentration values for the same species. The calculated ACR is applied to the acute aquatic toxicity

support staff conduct ASTER searches for EPA projects. The public has access to AQUIRE data through EPA's ECOTOX database at <http://www.epa.gov/ecotox/>, but the ECOTOX database does not screen the data.

criterion or toxic effect level selected for the pollutant of concern. EPA uses this method when an ACR is available for a species that has a measured chronic toxicity concentration greater than the acute criterion or the representative acute toxic effect level for the selected pollutant. These instances arise when chronic toxicity test data are available for less sensitive species only. The acute aquatic toxic effect level (used if national acute water quality criteria are not available) is typically the lowest reported acute aquatic bioassay test concentration (24- to 96-hour median lethal concentration, or LC₅₀) for a North American resident species of fish or invertebrate. As with chronic toxic effect levels, a test result of good quality is selected ahead of a test result of unknown quality.

The second option for estimating a chronic toxicity test concentration is to use ERL-Duluth's quantitative structure-activity relationship (QSAR) model. QSAR derives statistically based relationships between physical-chemical properties and biological activity. The QSAR model uses measured toxicity test results for compounds with similar chemical structures and properties to estimate MATC values for compounds whose chemical structure and properties are known or may be estimated.

The final option for estimating a chronic toxicity concentration is to apply an assumed ACR of 10:1 to the acute aquatic toxic effect concentration. The ACR of 10:1 is based on a recommendation in the EPA Office of Water's *Technical Support Document for Water Quality-based Toxics Control* (EPA, 1991) for estimating chronic toxicity when no data are available. The recommendation assumes that the chronic toxicity value is 10 times lower than the acute value.

2.4 REFERENCES

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SECTION 3

DIOXIN AND CONGENERS

EPA updated the TWFs for dioxin and its congeners to be consistent with EPA's ongoing assessment (EPA, 2003b). The revisions incorporate World Health Organization (WHO) Toxicity Equivalency Factors (TEFs) to adjust the cancer slope factors ($q1^*s$) and a derivation of BAFs. These are discussed in detail below.

3.1 SLOPE FACTORS AND TEFs

The Engineering and Analysis Division (EAD) continues to use the 1985 slope factor for tetrachlorodibenzo-*p*-dioxin, 2,3,7,8 (TCDD) in calculating TWFs. The 1985 slope factor of TCDD is $160,000 \text{ (mg/kg/d)}^{-1}$ (EPA, 1985). The slope factors of the other congeners are estimated by multiplying the slope factor of TCDD by the respective TEF. In accordance with EPA (2003b), EAD used the 1998 WHO TEFs to adjust the 1985 slope factors (Van den Berg et al., 1998). Table 3-1 gives the CAS numbers, names, and TEFs for the 17 congeners.

The revised slope factors are used to calculate updated human health values and the corresponding TWFs. The toxic equivalency value is calculated as follows:

$$= 1.6 \times 10^5 \text{ (slope factor)} \times \text{TEF}$$

For example, for hexachlorodibenzo-*p*-dioxin, 1,2,3,7,8,9, the toxic equivalency value is calculated as follows:

$$\begin{aligned} &= 1.6 \times 10^5 \text{ (slope factor)} \times 0.1 \text{ (TEF)} \\ &= 1.6 \times 10^4 \end{aligned}$$

Table 3-1
Dioxins and Their Toxic Equivalency Factors

CAS Number	Chemical Name	Abbreviated Name	Toxic Equivalency Factor
CDDs			
1746-01-6	tetrachlorodibenzo-p-dioxin, 2,3,7,8	TCDD, 2,3,7,8	1
40321-76-4	pentachlorodibenzo-p-dioxin, 1,2,3,7,8	PeCDD, 1,2,3,7,8	1
39227-28-6	hexachlorodibenzo-p-dioxin, 1,2,3,4,7,8	HxCDD, 1,2,3,4,7,8	0.1
57653-85-7	hexachlorodibenzo-p-dioxin, 1,2,3,6,7,8	HxCDD, 1,2,3,6,7,8	0.1
19408-74-3	hexachlorodibenzo-p-dioxin, 1,2,3,7,8,9	HxCDD, 1,2,3,7,8,9	0.1
35822-46-9	heptachlorodibenzo-p-dioxin, 1,2,3,4,6,7,8	HpCDD, 1,2,3,4,6,7,8	0.01
3268-87-9	octachlorodibenzo-p-dioxin, 1,2,3,4,6,7,8,9	OCDD, 1,2,3,4,6,7,8,9	0.0001
CDFs			
51207-31-9	tetrachlorodibenzofuran, 2,3,7,8	TCDF, 2,3,7,8	0.1
57117-41-6	pentachlorodibenzofuran, 1,2,3,7,8	PeCDF, 1,2,3,7,8	0.05
57117-31-4	pentachlorodibenzofuran, 2,3,4,7,8	PeCDF, 2,3,4,7,8	0.5
70648-26-9	hexachlorodibenzofuran, 1,2,3,4,7,8	HxCDF, 1,2,3,4,7,8	0.1
57117-44-9	hexachlorodibenzofuran, 1,2,3,6,7,8	HxCDF, 1,2,3,6,7,8	0.1
72918-21-9	hexachlorodibenzofuran, 1,2,3,7,8,9	HxCDF, 1,2,3,7,8,9	0.1
60851-34-5	hexachlorodibenzofuran, 2,3,4,6,7,8	HxCDF, 2,3,4,6,7,8	0.1
67562-39-4	heptachlorodibenzofuran, 1,2,3,4,6,7,8	HpCDF, 1,2,3,4,6,7,8	0.01
55673-89-7	heptachlorodibenzofuran, 1,2,3,4,7,8,9	HpCDF, 1,2,3,4,7,8,9	0.01
39001-02-0	octachlorodibenzofuran, 1,2,3,4,6,7,8,9	OCDF, 1,2,3,4,6,7,8,9	0.0001

Source: Van den Berg, et al., 1998.

3.2 BAFs

For dioxin and its congeners, EPA estimated BAFs based on the work done for the Great Lakes Water Quality Initiative (EPA, 1995). The BAFs in Table 10 of EPA's document are lipid normalized and freely dissolved based BAFs, also known as "Baseline BAFs," and were developed according to the methodology in EPA (2003c). This process of lipid-normalization and freely dissolved adjustment essentially "converts" the "site-specific" BAFs (derived from salmonids in the Great Lakes that have specific lipid and organic carbon content) into values that are ready for extrapolation to other conditions—that is, a national BAF.

The first step is to convert the BAFs from EPA (1995) to “Baseline BAFs” using the national defaults for f_l (fraction lipid) and f_{fd} (fraction dissolved) and the following equation:

$$\text{National BAF}_{TL\ n} = [(\text{Final Baseline BAF})_{TL\ n} \times (f_l)_{TL\ n} + 1] \times f_{fd}$$

where:

Final Baseline BAF_{TL n} = mean baseline BAF for trophic level (TL) n
 $(f_l)_{TL\ n}$ = fraction of tissue that is lipid in aquatic organisms at trophic level n
 f_{fd} = fraction of the total concentration of chemical in water that is freely dissolved

The national default trophic level–specific lipid fractions $(f_l)_{TL\ n}$ (where f_l = fraction lipid at TL n) are taken from EPA (2003c). These are shown in Table 3-2.

Table 3-2
National Default Values for Lipid Fractions by Trophic Level

Trophic Level	National Default Value
2	1.9%
3	2.6%
4	3.0%

Source: EPA, 2003c.

The f_{fd} (fraction freely dissolved) is calculated as follows:

$$f_{fd} = \frac{1}{1 + \text{POC} \times K_{ow} + \text{DOC} \times 0.08 \times K_{ow}}$$

where:

f_{fd} = fraction of the total concentration of chemical in water that is freely dissolved
POC = concentration of particulate organic carbon in water (kilograms of particulate organic carbon per liter of water)

DOC = concentration of dissolved organic carbon in water (kilograms of dissolved organic carbon per liter of water)

K_{ow} = *n*-octanol-water partition coefficient

The national default values for POC and DOC are 0.5 mg/L and 2.9 mg/L, respectively. The derivation of these values is explained in Section 6.3 of EPA (2003c).

For example, the BAF for TCDD, 2,3,7,8 is 9.00×10^6 for TL 4 (salmonids); and the $\log K_{ow}$ is 7.02 (EPA, 1995). Given these two parameters, we can calculate the national BAF for a given trophic level. The first step is to calculate the fraction of the total concentration of TCDD, 2,3,7,8 that is freely dissolved:

$$f_{fd} = \frac{1}{1 + \text{POC} \times K_{ow} + \text{DOC} \times 0.08 \times K_{ow}}$$

where:

POC = 5.0×10^{-7} kg/L (national default values)

DOC = 2.9×10^{-6} kg/L (national default values)

Log K_{ow} = 7.02 (that is, $K_{ow} = 10^{7.02}$, which, in turn, equals 10,471,285)

so:

$$f_{fd} = \frac{1}{1 + 5.0 \times 10^{-7} \text{ kg/L} \times 1.05 \times 10^7 + 2.9 \times 10^{-6} \text{ kg/L} \times 0.08 \times 1.05 \times 10^7}$$

$$f_{fd} = 1.1541 \times 10^{-1}$$

The next step is to insert this value for the freely dissolved fraction of TCDD, 2,3,7,8 into the following equation:

$$\text{National BAF}_{TL\ n} = [(\text{Final Baseline BAF})_{TL} * (f_l)_{TL\ n} + 1] * f_{fd}$$

where:

Final Baseline $\text{BAF}_{TL\ n}$ = 9.00×10^6 for TL 4

$$\begin{aligned}(f_l)_{TL\ n} &= 0.03 \text{ for TL 4} \\ f_{fd} &= 1.1541 \times 10^{-1}\end{aligned}$$

so:

$$\begin{aligned}\text{National BAF}_{TL\ 4} &= [(9.00 \times 10^6)_4 \times (.03)_4 + 1] \times 1.1541 \times 10^{-1} \\ \text{National BAF}_{TL\ 4} &= 3.1160 \times 10^4\end{aligned}$$

EPA did not have BAF data for TLs 2 and 3 for dioxin. Therefore, all of the 17.5 grams/day fish consumption was apportioned to TL 4.

Using the equation shown in Table 2-1 for carcinogenicity protection (organism only), we obtain:

$$HHOO \text{ (ug / L)} = \frac{\left(\frac{(10^{-5})}{160,000} \right) \times 70 \text{ kg} \times 1,000 \text{ ug / mg}}{0.0175 \text{ kg / day} \times (3.1160 \times 10^4 \times (\text{L / kg}))}$$

or

$$HHOO \text{ (ug/L)} = 8.02 \times 10^{-9}$$

The toxic weighting factor would be calculated using the following equation:

$$TWF = \frac{5.6}{1.0 \times 10^{-6}} + \frac{5.6}{8.02 \times 10^{-9}}$$

or TWF for TCDD, 2,3,7,8 is 7.04×10^8 .

3.3 REFERENCES

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SECTION 4

DEVELOPMENT OF TWF DATABASE

4.1 DATABASE OVERVIEW

In May 2004, EPA decided to develop a database to support the transparency, reproducibility, and documentation of TWF values. The database is in Excel™ and can be found in the docket.

The overall organization of the individual sheets within the file is as follows:

- Read First: Instructions on using the model.
- Data Dictionary: List of variable names, with definitions and sources for the data.
- TWFs: Master list of TWFs. Human health values based on carcinogens are converted to a 10^{-5} risk level, human and aquatic health values are standardized to the value for copper (5.6 µg/L), preferred human and aquatic health values are identified and added.
- HH_CALC: Calculated human health value for carcinogens and non-carcinogens for organisms only and water and organisms. All variables are linked to data sheets by Chemical Abstracts Service (CAS) number.
- AQ_FRESH_ACUTE: What the acute aquatic health values for freshwater species are based on (e.g., LC_{50} , species, and citation). If the data are taken from ASTER, the original reference is included. Separate columns track the source date, last reviewed date, and last update date.
- AQ_FRESH_CHRONIC: Counterpart to AQ_FRESH_ACUTE for chronic exposures.
- AQ_SALT_ACUTE: Counterpart to AQ_FRESH_ACUTE for saltwater species.
- AQ_SALT_CHRONIC: Counterpart to AQ_SALT_ACUTE for chronic exposures.
- BCF_BAF: Data sheet for BCFs and BAFs, study duration, species, and citation. Separate columns track the source date, last reviewed date, and last update date.
- Cancer_Potency_Factor: Cancer potency factor values—also called cancer slope factors, slope factors, or q_1^* —and citations. Separate columns track the source date, last reviewed date, and last update date.
- Reference Dose: Contains each RfD's value, citation, and three columns tracking the date of the source, last review, and last update.

- Relative Source Contribution: A parameter that adjust the human health value for ingestion of aquatic organisms to account for exposure from other sources. Contains value, citation, and three columns tracking the date of the source, last review, and last update.
- Constants: For example, fish intake for calculating the human health criteria.

The purpose of the database is to duplicate the TWFs in use by EPA in a self-contained database whose reader can track the data from the original sources through all of the calculations to the final TWF value. As mentioned in Section 1, the set of approximately 1,900 TWF values grew over the course of several decades. The output of the August 2004 database was compared against a master list of TWF values and no discrepancies were found. EPA proceeded with its industry analysis for the 304(m) process with the August 2004 data while it began an overall review and update of the database according to the needs outlined in Zipf (2003). These updates are discussed in Section 5.

4.2 QUALITY CONTROL REVIEWS

EPA used the structure of the new TWF database to facilitate a series of quality control reviews. These included searching for:

- Missing references for any of the parameters.
- Unknown codes for any of the parameters.
- Missing species for any of the aquatic health values.
- No adjustment on the carcinogenicity risk values to 10^{-5} risk level (i.e., values that should have been adjusted from a 10^{-6} risk level to a 10^{-5} risk level but were not).
- Acute:chronic ratios for aquatic health not adjusted to 1991 value of 10.
- Corrections to references.
- Pollutants whose TWFs were calculated on either the human health or aquatic health data when EPA had data for both parameters.
- Pollutants for which no TWF was calculated when EPA had data for at least one of the human or aquatic health parameters.

The results of the quality control reviews were summarized in a memo to the project files (ERG, 2004).

4.3 REFERENCES

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SECTION 5

UPDATED TWF DATABASE

The updates to the TWF database were completed in December 2004. EPA then compared the August and December TWF values. Of the approximately 1,900 pollutants, about 1,450 showed no change between the August and December databases. Another 372 TWFs registered as showing a change in value due to a shift to the 2000 human health methodology (“2000 methodology”), but the differences were so small ($10e-7$ to $10e-19$ in value) as to be negligible. Table 5-1 lists TWFs for 26 pollutants for which the change to the 2000 methodology resulted in a change of at least 1 percent in the value of the TWF. An additional 54 TWFs changed due to updated data. This group includes dioxin and its congeners; the group is presented in Table 5-2.

When comparing the August and December 2004 values, EPA noticed that one pollutant—manganese—no longer had a value. Manganese is anomalous in that EPA (2002) provides a recommended human health value but does not provide any of the underlying components used to calculate it. For manganese, then, the human health value is hard-wired instead of being calculated from its component parts.

5.1 REFERENCE

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Table 5-1
Comparison of August and December 2004 TWF Values
Changes Due to Shift to 2000 Methodology

Pollutant	CAS Number	TWF Values		Difference	Difference as a Percent
		December	August		
Dichloropropene, trans-1,3-	10061026	2.30e-02	2.33e-02	-3.97e-04	-1.73%
Dichloropropene, cis-1,3-	10061015	2.30e-02	2.33e-02	-3.97e-04	-1.73%
Dichloropropene, 1,3-	542756	5.65e-01	5.42e-01	6.57e-03	1.16%
Thallium	7440280	1.03e+00	1.00e+00	2.53e-02	2.47%
Allyl chloride	107051	3.35e-03	2.91e-03	1.16e-04	3.47%
Chlorine	7782505	5.09e-01	4.87e-01	2.21e-02	4.35%
Tribromomethane	75252	4.57e-03	1.75e-03	2.10e-04	4.59%
Trichloroethene	79016	1.91e-02	6.44e-03	8.82e-04	4.62%
Simazine	122349	6.42e-01	5.61e-01	3.01e-02	4.68%
BHC, gamma-/lindane	58899	7.03e+01	4.69e+01	8.56e+00	12.18%
Dinitrotoluene, 2,4-	121142	4.45e-01	2.81e-01	6.05e-02	13.57%
Arsenic	7440382	4.04e+00	3.47e+00	5.72e-01	14.15%
Nitrosopyrrolidine, –	930552	1.62e-02	3.28e-03	2.73e-03	16.88%
Chrysene	218019	3.10e+01	2.10e+00	9.63e+00	31.07%
Indeno(1,2,3-cd)pyrene	193395	3.07e+01	1.14e+00	1.02e+01	33.43%
Tetrachloroethene	127184	2.34e-01	1.26e-02	8.12e-02	34.72%
Atrazine	1912249	2.31e+00	9.44e-02	8.23e-01	35.60%
Pentachloronitrobenzene/ Quintozone	82688	3.85e+01	7.41e-01	1.39e+01	36.13%
Alachlor/Lasso	15972608	1.78e+00	1.57e-02	6.49e-01	36.52%
Aldrin	309002	1.11e+04	5.02e+01	4.10e+03	36.84%
Parachlorometacresol	59507	1.33e+00	4.33e-03	4.93e-01	37.02%
Chlorobenzilate	510156	7.92e+01	1.56e-01	2.93e+01	37.03%
Trichloropropane, 1,2,3-	96184	5.26e+00	1.96e-03	1.95e+00	37.11%
Hydrofluoric acid	7664393	5.60e-06	0.00e+00	2.08e-06	37.14%
Aflatoxins	4402682	1.79e+04	0.00e+00	6.64e+03	37.14%
Azinphos methyl/ Guthion, methyl-	86500	5.61e+01	2.80e+01	2.80e+01	49.93%
Cadmium	7440439	2.31e+01	2.61e+00	1.99e+01	85.89%
Ethoprophos	13194484	8.89e+01	3.81e-01	8.85e+01	99.57%

Source: EPA estimates.

Table 5-2
Changes in TWFs Due to Updates

Pollutant	CAS Number	TWF		Reasons for Differences
		December	August	
Tetrachlorodibenzo-p-dioxin, 2,3,7,8-	1746016	7.04E+08	4.22E+08	Dioxin congener: change from BCFs to BAFs
Pentachlorodibenzo-p-dioxin, 1,2,3,7,8-	40321764	6.93E+08	2.15E+08	Dioxin congener: change from BCFs to BAFs
Hexachlorodibenzo-p-dioxin, 1,2,3,7,8,9-	19408743	1.06E+07	4.31E+07	Dioxin congener: change from BCFs to BAFs
Hexachlorodibenzo-p-dioxin, 1,2,3,4,7,8-	39227286	2.35E+07	4.31E+07	Dioxin congener: change from BCFs to BAFs
Hexachlorodibenzo-p-dioxin, 1,2,3,6,7,8-	57653857	9.56E+06	4.18E+07	Dioxin congener: change from BCFs to BAFs
Pentachlorodibenzofuran, 2,3,4,7,8-	57117314	5.57E+08	3.29E+07	Dioxin congener: change from BCFs to BAFs
Tetrachlorodibenzofuran, 2,3,7,8-	51207319	4.38E+07	6.70E+06	Dioxin congener: change from BCFs to BAFs
Hexachlorodibenzofuran, 1,2,3,7,8,9-	72918219	4.73E+07	6.67E+06	Dioxin congener: change from BCFs to BAFs
Hexachlorodibenzofuran, 1,2,3,6,7,8-	57117449	1.41E+07	6.67E+06	Dioxin congener: change from BCFs to BAFs
Hexachlorodibenzofuran, 1,2,3,4,7,8-	70648269	5.76E+06	6.66E+06	Dioxin congener: change from BCFs to BAFs
Hexachlorodibenzofuran, 2,3,4,6,7,8-	60851345	5.12E+07	6.66E+06	Dioxin congener: change from BCFs to BAFs
Heptachlorodibenzo-p-dioxin, 1,2,3,4,6,7,8-	35822469	4.11E+05	4.18E+06	Dioxin congener: change from BCFs to BAFs
Pentachlorodibenzofuran, 1,2,3,7,8-	57117416	7.63E+06	3.29E+06	Dioxin congener: change from BCFs to BAFs
Heptachlorodibenzofuran, 1,2,3,4,7,8,9-	55673897	3.03E+06	6.67E+05	Dioxin congener: change from BCFs to BAFs
Heptachlorodibenzofuran, 1,2,3,4,6,7,8-	67562394	8.58E+04	6.66E+05	Dioxin congener: change from BCFs to BAFs
Octachlorodibenzo-p-dioxin	3268879	6.59E+03	4.24E+05	Dioxin congener: change from BCFs to BAFs
Octachlorodibenzofuran	39001020	2.02E+03	6.74E+04	Dioxin congener: change from BCFs to BAFs
Dieldrin	60571	1.06E+04	5.67E+04	BCF changed; new value taken from EPA, 2002
Benzo(a)pyrene	50328	1.01E+02	4.28E+03	BCF changed; new value taken from EPA, 2002
Dibenzo(a,h)anthracene	53703	3.07E+01	1.69E+03	BCF changed; new value taken from EPA, 2002
Benzo(b)fluoranthene	205992	3.07E+01	4.21E+02	BCF changed; new value taken from EPA, 2002
Benzo(a)anthracene	56553	3.63E+01	1.81E+02	BCF changed; new value taken from EPA, 2002
Mercury	7439976	1.17E+02	1.17E+02	BCF changed; new value taken from EPA, 2002
Benzo(k)fluoranthene	207089	3.07E+01	4.21E+01	BCF changed; new value taken from EPA, 2002
Nitrosodi-n-butylamine, –	924163	2.56E+00	4.77E+00	BCF changed; new value taken from EPA, 2002

Table 5-2
Changes in TWFs Due to Updates

Pollutant	CAS Number	TWF		Reasons for Differences
		December	August	
Nitrosodi-n-propylamine, –	621647	1.11E+00	2.29E+00	BCF changed; new value taken from EPA, 2002
Aniline	62533	6.86E-03	1.41E+00	BCF changed; new value taken from ASTER
Pentachlorobenzene	608935	3.77E+00	2.26E+00	BCF changed; new value taken from EPA, 2002
Vanadium	7440622	3.50E-02	6.22E-01	Aquatic health value changed; new values taken from ASTER
Dibromochloromethane	124481	4.45E-02	1.27E-01	BCF changed; new value taken from EPA, 2002
Trichlorophenol, 2,4,6-	88062	4.98E-01	4.44E-01	BCF changed; new value taken from EPA, 2002
Bromodichloromethane	75274	3.29E-02	7.42E-02	BCF changed; new value taken from EPA, 2002
Trichlorobenzene, 1,2,4-	120821	2.55E-02	8.21E-02	BCF changed; new value taken from EPA, 2002
Manganese	7439965	1.44E-02	7.04E-02	TWF database will be updated to include human health values
Chloroethene	75014	8.55E-02	1.16E-01	q1* changed; new value taken from IRIS
Pyrene	129000	9.32E-02	1.11E-01	BCF changed; new value taken from EPA, 2002
Trichlorophenol, 2,4,5-	95954	1.78E-02	2.62E-02	BCF changed; new value taken from EPA, 2002
Ethylenethiourea	96457	1.56E-01	6.71E-02	q1* changed, see memo “Fixes to Toxic Weighting Factor (TWF) Data” from Maureen Kaplan, ERG, to Lynn Zipf, EPA, dated November 1, 2004
Beryllium	7440417	1.06E+00	1.06E+00	BCF changed; new value taken from EPA, 2002
Nitrophenol, 4-	100027	4.89E-03	9.44E-03	BCF changed; new value taken from EPA, 2002
Fluorene	86737	7.01E-01	7.04E-01	BCF changed; new value taken from EPA, 2002
Chloronaphthalene, 2-	91587	2.16E-02	2.23E-02	BCF changed; new value taken from EPA, 2002
Anthracene	120127	2.55E+00	2.55E+00	BCF changed; new value taken from EPA, 2002
Ammonia as N	7664417	1.35E-03	1.83E-03	Fresh acute value changed; value taken from 1999 update of ambient water quality for ammonia

Table 5-2
Changes in TWFs Due to Updates

Pollutant	CAS Number	TWF		Reasons for Differences
		December	August	
Dichloroethene, 1,2-	540590	1.46E-03	1.27E-03	Oral reference dose changed; see memo "Fixes to Toxic Weighting Factor (TWF) Data" from Maureen Kaplan, ERG, to Lynn Zipf, EPA, dated November 1, 2004
Bromomethane	74839	5.98E-02	5.77E-02	BCF changed; new value taken from EPA, 2002
Dichloropropane, 1,2-	78875	3.94E-02	1.55E-02	BCF changed; new value taken from EPA, 2002
Hexachlorobutadiene	87683	6.33E-01	6.14E-01	BCF changed; new value taken from EPA, 2002
Benzene	71432	3.17E-02	1.84E-02	BCF changed; new value taken from EPA, 2002
Dimethylphenol, 2,4-	105679	9.41E-03	5.29E-03	BCF changed; new value taken from EPA, 2002
Dichloromethane	75092	1.01E-03	4.23E-04	BCF changed; new value taken from EPA, 2002
Dinitrophenol, 2,4-	51285	8.14E-03	7.48E-03	BCF changed; new value taken from EPA, 2002
Dichloroethene, trans-1,2-	156605	9.20E-05	9.25E-05	BCF changed; new value taken from EPA, 2002
Bis(2-chloroisopropyl) ether	108601	2.54E-02	1.26E-03	BCF changed; new value taken from EPA, 2002

Source: EPA estimates.

SECTION 6

TWF DEVELOPMENT

As EPA continues to study different industries and their discharges as reported to TRI and PCS, there is a periodic need to review, update, and/or develop TWFs for specific chemicals or groups of chemicals. Appendix A contains the data sheets developed for summarizing the information available. After EPA's internal review, these will be incorporated in the next release of the TWF database. Section 6.1 discusses updates requested in the fall of 2004. Sections 6.2 through 6.5 provide background information on the development of TWFs for methylmercury, polycyclic aromatic compounds (PACs), nitrogen, and the second list of drinking water contaminants published by EPA on February 24, 2005 (EPA, 2005a).

6.1 FALL 2004 LIST OF CHEMICALS

In October 2004, EPA decided to review, update, and/or develop TWFs for:

- Hydrogen fluoride, CAS 7664393
- Chlorine dioxide, CAS 10049044
- 1,3-phenylenediamine, CAS 108452
- Benzo(a)pyrene, CAS 50328
- Aniline, CAS 62533
- Vanadium, CAS 7440622

The worksheets are shown in Appendices A-2 through A-7.

6.2 METHYLMERCURY

EPA (2002a) presents a human health water quality criterion for methylmercury expressed as a fish and shellfish tissue concentration. The criteria for all other contaminants are expressed as water column concentrations. EPA also presented the RSC for methylmercury as an amount subtracted from the RfD, rather than as a percentage as is done with the other contaminants.

For the TWF database, however, EPA needs to convert water quality criterion from a methylmercury concentration in fish tissue to a methylmercury concentration in water. EPA also needs to convert the RSC to a percentage for use in the TWF database. The first conversion is discussed in Section 6.2.1 while the second is presented in Section 6.2.2. The data sheets for mercury and methylmercury are located in Appendix A-8 and A-9, respectively.

6.2.1 Water Quality Criterion for Methylmercury as a Concentration in Water

In a *Federal Register* notice (EPA, 2001a), EPA provided three approaches to relate the methylmercury fish tissue water quality criterion to a concentration of methylmercury in the water column. The first approach is to collect site-specific BAFs based on water and fish collected in the waterbody of concern. This approach is not appropriate for a national-level analysis. The second approach is to use a bioaccumulation model with site-specific parameters. Again, the site-specific nature of the approach is not appropriate for a national-level analysis.

The third approach is to use empirically derived draft BAFs.⁵ These are national estimates. The *Federal Register* notice's data for fish intake (FI) by trophic level and BAF by trophic level were used to create a weighted-average national BAF for methylmercury for the purpose of estimating a TWF for the 304(m) process. Table 6-1 reproduces the calculations. For each trophic level, the product of the BAF and the FI are used. For example, for trophic level 2, the product of 1.6×10^5 BAF and .0038 (kg/day) FI is 608. The calculation is repeated for trophic levels 3 and 4. The final column in Table 1 is the sum of the FIs (0.0175 kg/day) and the product of the BAFs (21,438). Dividing 21,438 by the total FI (0.0175) estimates the weighted-average BAF value of 1.225029×10^6 .

⁵Final methylmercury BAFs were not found in the *Federal Register* for 2001 through November 2004 .

Table 6-1
Weighted-Average National BAF for Methylmercury

Parameter	Trophic Level			Sum
	2	3	4	
Bioaccumulation factor	1.60e+05	6.80e+05	2.70e+06	
Fish intake (kg/day)	3.80e-03	8.00e-03	5.70e-03	1.75e-02
Product: BAF(trophic level) × FI(trophic level)	6.08e+02	5.44e+03	1.54e+04	2.14e+04
Weighted average BAF				1.23e+06

Source: EPA, 2001.

6.2.2 Conversion of RSC from a Value to be Subtracted to a Percentage

EPA (2001a) presents the RSC as an amount to be subtracted rather than a percentage. The equations in the TWF model assume the RSC is a percentage. Table 6-2 shows the conversion calculations. The RfD for methylmercury is 0.1 µg/kg/day (66 FR 1353), or 0.0001 mg/kg/day. The RSC in the subtraction approach is 2.7×10^{-5} , or 0.000027 mg/kg/day (66 FR 1354). The difference between the RfD and the RSC, i.e., the amount to be multiplied by body weight in the water quality criterion calculations, is 7.25×10^{-5} , or 0.0000725. Dividing 0.0000725 by 0.0001 equals 0.725. The equivalent value for RSC is 73 percent.

Table 6-2
Conversion of RSC from Amount Subtracted to Percentage

Parameter	Value
RfD (mg/kg BW-day)	0.0001000
RSC (mg/kg BW-day)	0.0000275
Difference	0.0000725
(RfD-RSC)/RfD = RSC as a percentage of RfD	0.7250000

Source: EPA estimates.

6.3 POLYCYCLIC AROMATIC COMPOUNDS

6.3.1 Background

Table 6-3 lists the 21 chemicals considered to be PACs, based on the Emergency Planning and Community Right-To-Know Act guidance as of August 2001 (EPA, 2001b). Most of these compounds are the product of incomplete combustion or are from fossil fuels. Two of these chemicals—dimethylbenz(a)anthracene, 7, 12 and methylcholanthrene, 3—have been produced in small quantities as research chemicals. They are listed in EPA (2001b) as formed during combustion. Understandably, no human health or aquatic life data are available for these two chemicals and they are excluded from further discussion in this memorandum.

Section 6.3.2 reviews the chemicals for which EPA has already developed human health water quality criteria using the 2000 methodology. Section 6.3.3 summarizes the availability of aquatic life values for the PACs listed in Section 6.3.2. Section 6.3.4 discusses the human and aquatic health data available for the remaining chemicals. Section 6.3.5 summarizes the findings and proposes a general PAC TWF. Worksheets for each chemical are located in Appendix A-5 and A-10 through A-27.

6.3.2 Human Health

EPA (2002a) published water quality criteria for:

- Benzo(a)anthracene
- Benzo(a)phenanthrene (chrysene)
- Benzo(a)pyrene
- Benzo(b)fluoranthene
- Benzo(k)fluoranthene
- Benzo(j,k)fluorene (fluoranthene)
- Dibenzo(a,h)anthracene
- Indeno(1,2,3-cd)pyrene

EPA (2002b) also noted that the IRIS value for benzo(b)fluoranthene (CAS 205992) was used to derive the value presented for benzo(a)anthracene, benzo(a)phenanthrene (chrysene), benzo(k)fluoranthene,

Table 6-3
Chemicals Included in the EPCRA Section 313 PAC Category

Chemical Name	CAS Number
Benzo(a)anthracene	56553
Benzo(a)phenanthrene (chrysene)	218019
Benzo(a)pyrene	50328
Benzo(b)fluoranthene	205992
Benzo(j)fluoranthene	205823
Benzo(k)fluoranthene	207089
Benzo(j,k)fluorene (fluoranthene)	206440
Benzo(r,s,t)pentaphene	189559
Dibenz(a,h)acridine	226368
Dibenz(a,j)acridine	224420
Dibenzo(a,h)anthracene	53703
Dibenzo(a,e)fluoranthene	5385751
Dibenzo(a,e)pyrene	192654
Dibenzo(a,h)pyrene	189640
Dibenzo(a,l)pyrene	191300
7H-dibenzo(c,g)carbazole	194592
7,12-dimethylbenz(a)anthracene	57976
Indeno(1,2,3-cd)pyrene	193395
3-methylcholanthrene	56495
5-methylchrysene	3697243
1-nitropyrene	5522430

Source: EPA, 2001b.

dibenzo(a,h)anthracene, and indeno(1,2,3-cd)pyrene. As such, data are truly only available for three chemicals:

- Benzo(a)pyrene
- Benzo(b)fluoranthene
- Benzo(j,k)fluorene (fluoranthene)

6.3.3 Aquatic Life Criteria

EPA (2002a) did not publish corresponding aquatic life criteria for the eight PACs listed in Section 6.3.2. ASTER data were reviewed in order to identify appropriate studies and values for deriving aquatic life criteria. ASTER sometimes reports studies in two separate sections—the first section includes studies that pass ASTER’s filter for data of the highest quality and the second section includes studies that do not pass the filter for data quality but are included in the AQUIRE (now ECOTOX) database. A researcher with access only to ECOTOX would not have identified better data sources.

Where possible, data that passed the ASTER filter were used. In addition, data were not used—even if they passed the filter—if the citation was a personal communication. With these two criteria, higher concentrations than those cited in the earlier TWF data were identified. That is, both citations appear in ECOTOX, but the study that ASTER identified as being of higher quality was used. Table 6-4 summarizes these changes.

Table 6-4
Changes to Aquatic Life Health Data

Chemical	Aquatic Life Category	Values (µg/L)	
		Old	New
Benzo(a)anthracene	Fresh-acute	10	1,599
Benzo(a)anthracene	Fresh-chronic	1	160
Benzo(a)phenanthrene chrysene	Fresh-acute	592	1,599
Benzo(a)phenanthrene chrysene	Fresh-chronic	16	160
Benzo(j,k)fluorene (fluoranthene)	Fresh-chronic	7.1	4.5
Dibenzo(a,h)anthracene	Fresh-acute	NA	496
Dibenzo(a,h)anthracene	Fresh-chronic	NA	50

Source: ASTER, 2004.

6.3.4 Remaining Chemicals

The remaining PACS for which no water quality criteria were available are:

- Benzo(j)fluoranthene
- Benzo(r,s,t)pentaphene
- Dibenz(a,h)acridine
- Dibenz(a,j)acridine
- Dibenzo(a,e)fluoranthene
- Dibenzo(a,e)pyrene
- Dibenzo(a,h)pyrene
- Dibenzo(a,l)pyrene
- 7H-dibenzo(c,g)carbazole
- 5-methylchrysene
- 1-nitropyrene

No human health criteria were found for these 11 chemicals in IRIS, the EPA Region 3 RBC Table, ATSDR toxicological profiles, the EPA 2000 Water Quality Standards, or the EPA 1995 Final Water Quality Guidance for the Great Lakes System. ASTER data were examined for these chemicals, and only data for 7H-dibenzo(c,g)carbazole were found.

6.3.5 Summary and Proposed PAC TWFs

For the human health component of the PAC TWF, values were identified for three chemicals: benzo(a)pyrene, benzo(b)fluoranthene, and benzo(j,k)fluoranthene. The first two are carcinogens and have the same cancer slope value ($q1^* = 7.3 \text{ mg/kg/day}$). The third is a non-carcinogen with a RfD of 0.04 mg/kg/day . After adjusting the cancer risk factor to 10^{-5} and standardizing the PACs to copper, the human health, organism-only component for the TWF range is nearly three orders of magnitude, as follows:

- benzo(a)pyrene: 30.7
- benzo(b)fluoranthene: 30.7
- benzo(j,k)fluoranthene: 0.0403

Aquatic life data were identified for 6 of the 21 PACs. These data are summarized in Table 6-5.

Table 6-5
Aquatic Health Data for PAC Chemicals

Chemical	Fresh		Salt	
	Chronic	Acute	Chronic	Acute
Benzo(a)anthracene	160	1,599	7.5	75
Benzo(a)phenanthrene (chrysene)	160	1,599		
Benzo(a)pyrene	0.08	5	100	1,000
Benzo(j,k)fluorene (fluoranthene)	4.5	45		
7H-dibenzo(c,g)carbazole	185	1,852		
1-nitropyrene	215	2,149		
Dibenzo(a,h)anthracene	496	496	5	50
Geometric Mean ($\mu\text{g/L}$)	29.2	379.6	15.5	155.4
Toxic Weighting Factor Component Value	0.19	0.01	0.36	0.04

Source: ASTER, 2004.

EPA identified three approaches to developing TWFs for PACs. First, where the composition of the PAC discharge is known, EPA could separate the discharge into its constituents and calculate toxic-weighted pound-equivalents using the chemical-specific TWFs. Second, EPA could use the highest TWF

for any constituent within the PAC discharge—usually benzo(a)pyrene—as an upper-bound estimate of relative toxicity. The second approach, however, could mask a difference between two industrial discharges when one discharge is 100 percent benzo(a)pyrene and the second discharge is a PAC with a substantial fraction of benzo(j,k)fluoranthene.

The third approach is to estimate a TWF for a generalized PAC. The 304(m) screening process is just that: a nation-wide screening process, not a site- or discharge-specific risk assessment. In this case, EPA does not know the composition of the PAC discharge (e.g., 50 percent benzo(a)pyrene, 10% benzo(j,k)fluoranthene). There is no single known or suspected common mode of action shared by the class of compounds, that is, some PACs have a cancer mode of action while others are non-carcinogenic. This means that PACs do not meet the minimum data requirements for developing a relative potency factor (EPA, 2000).

Strictly for the purposes of ranking discharges for the 304(m) process, EPA considered developing a generalized PAC TWF. EPA considered several distributions and measures of central tendency and noted that:

- A three-order-of-magnitude range in human health values suggests that a logarithmic distribution might be the most appropriate assumption for the distribution of human health values.
- Logarithmic transformations are used to stabilize the variance if the standard deviation in the original scale varies with the mean (Snedcor and Cochran, 1980). That is, the effects are proportional.
- Both modes of operation (cancer and non-cancer) use the same risk level (10^{-5}).

The geometric mean for the copper-standardized human health component for benzo(a)pyrene, benzo(b)fluoranthene, and benzo(j,k)fluoranthene is the cube root of $(30.7 \times 30.7 \times 0.0403)$, or 3.36. The geometric mean for the copper-standardized chronic aquatic health criterion for fresh water is 0.19 (see Table 6-5). The proposed TWF for PACs is, therefore, 3.57—that is, the sum of 3.36 and 0.19.

6.4 NITROGEN

EPA decided to perform a comprehensive review of aquatic and human health data for nitrogen in various forms in order to provide a consistent and documented basis for the proposed TWFs. TRI and PCS report discharges for:

- Sodium nitrite
- Ammonia
- Nitrogen, total (as N)
- Nitrogen, Kjeldahl total (as N)
- Nitrogen oxides (as N)
- Nitrogen, organic total (as N)
- Nitrogen, nitrite total (as N)
- Nitrogen, inorganic total
- Nitrogen, Kjeldahl total (TKN)
- Nitrite nitrogen, dissolved (as N)
- Nitrogen, nitrite total (as NO₂)
- Nitrogen (as NO₃) sludge solid

For nitrogen, the sensitive population is an infant or small child and the major pathway is drinking water. Nitrite reacts with the ferrous iron in hemoglobin to form methemoglobin with iron in the ferric valence state. Ferric iron is unable to transport oxygen, leading to shortness of breath, skin turning blue, and oxygen deprivation in the brain. Although humans convert ingested nitrate into nitrite in the gut, the amount converted depends on several factors. The pH of the gut is normally higher in infants than in older children and adults, and the higher pH enhances nitrate-to-nitrite conversion. In addition, fetal hemoglobin is oxidized more readily by nitrite to methemoglobin, making infants and children the sensitive subpopulation (ATDSR, 2001; IRIS, 2004, 2005a).

The human health component of a TWF, however, is based on the exposure of an **adult** via organism only (not drinking water and organism; see Table 2-1 and Section 2.2). As IRIS (2005a) notes, nitrate is a normal component of the human diet. In addition, there is no oral RfD for ammonia reported in IRIS (IRIS, 2005b). For these reasons, **no human health component** is calculated for the various forms of nitrogen. The TWFs are based on aquatic health only.

6.4.1 Sodium Nitrite

Sodium nitrite is not included in the forms of organic nitrogen listed in APHA et al., 1995. It should not be surprising, then, that its TWF might differ substantially from those for components of the nitrogen cycle. Sodium nitrite was added to the list of chemicals reported in TRI in 1994 under the Emergency Planning and Community Right-to-Know Act (EPCRA) section 313(d)(2)(B) based on chronic hematological and developmental toxicity data from mouse and rat studies (EPA, 1994).

The ASTER report for sodium nitrite CAS 7632-00-0 references more than 120 studies. Only the studies that passed the ASTER filter were considered for the TWFs. The median acute data are:

- Rainbow trout, 96-hr LC₅₀: 150 µg/L
- Cutthroat trout, 96-hr LC₅₀: 560 µg/L
- Fathead minnow, 96-hr LC₅₀: 2,990 µg/L

The median chronic data are:

- Channel catfish, 31-day exposure, growth: 1,620 µg/L
- Channel catfish, 31-day exposure, mortality: 1,250 µg/L

What is apparent is that there is a wide range of sensitivity according to the species examined. Channel catfish are far less sensitive than rainbow trout; the median **chronic** values for catfish are about 10 times higher than the median **acute** value for rainbow trout. The sensitivity of salmonids is apparent for ammonia as well as sodium nitrite; see EPA (1999a) Figure 8, where the graphs for salmonids have a maximum value of 200 mg N/L, while the maximum values for other species range from 400 mg N/L to 2,000 mg N/L for catfish. See also EPA (1999a), Figure 11 and pages 40–41, concerning the sensitivity of salmonids to pollutants.

Within the acute data, a study of fathead minnows reported a 96-hour LC₅₀ acute value of 2,990 µg/L, a factor of 20 times higher than the 96-hour LC₅₀ acute value reported for rainbow trout of 150 µg/L.

EPA has four options for the sodium nitrite TWF. If EPA uses the lowest 96-hour LC_{50} acute value for a species and reduces it by an order of magnitude to produce the chronic value, the options are 15 $\mu\text{g/L}$ (rainbow trout), 56 $\mu\text{g/L}$ (cutthroat trout), and 299 $\mu\text{g/L}$ (fathead minnow). If EPA uses the chronic data for channel catfish, the value is 1,250 $\mu\text{g/L}$. EPA is proposing to use the 15 $\mu\text{g/L}$ value to protect the most sensitive species.

Finally, sodium nitrite is reported to TRI as pounds of sodium nitrite released. The aquatic health data are reported in $\mu\text{g/L}$ of sodium nitrite (not nitrogen). The discharges reported in TRI and the TWF for sodium nitrite are on the same basis.

6.4.2 Nitrogen Cycle Components

This discussion is based primarily on the information in *Standard Methods* (APHA et al., 1995). In order of increasing oxidation state, the forms of nitrogen in the cycle are:

- Organic nitrogen (organically bound nitrogen in the tri-negative oxidative state—includes urea, nucleic acids, peptides, and proteins)
- Ammonia
- Nitrite
- Nitrate

Some analyses are reported in terms of “Kjeldahl nitrogen” or TKN. TKN refers to ammonia plus organic nitrogen identified in a single analysis. It is named after J. Kjeldahl, who invented the analytic methods. The analysis results do not measure nitrogen in the form of nitrate, nitrite, nitrile, nitroso, onime, azide, aszine, azo, hydrazone, or semi-carbazone. “Total oxidized nitrogen” is the sum of nitrate and nitrite.

Nitrite is an intermediate oxidation state of nitrogen. Certain bacteria can oxidize ammonium to nitrite and then to nitrate. This happens rather quickly in aerobic environments such as receiving streams and dry soils. On the other hand, in an anoxic (reducing) environment such as bottom waters and saturated soils, certain bacteria can convert nitrate to nitrite and then further convert the nitrogen into gaseous forms (APHA et al., 1995; EPA, 2005b, 2005c).

6.4.2.1 Ammonia

EPA's 1999 *Update of Ambient Water Quality Criteria for Ammonia* (EPA, 1999a) states that the limits are given "in terms of nitrogen, i.e., as mg N/L, because most permit limits for ammonia are expressed in terms of nitrogen." In aqueous solutions, ammonia exists in equilibrium in two forms—un-ionized ammonia (NH_3) and ammonium ion (NH_4^+).⁶ Un-ionized ammonia is the more toxic component. TRI guidance for reporting discharges of aqueous ammonia recommends that total aqueous ammonia be calculated in terms of un-ionized ammonia equivalents (TRI, 2000a).

The criteria vary as a function of pH, temperature, and whether early life stages are present. For the purpose of evaluating the toxicity of industrial wastewater discharges, we assumed that early life stages were present, pH = 7, and temperature = 20 degrees Celsius. The chronic criterion under these circumstances is 4,150 $\mu\text{g N/L}$. If we change the assumed pH to 8, the criterion drops to 1,710 $\mu\text{g N/L}$.

The ammonia-as- NH_3 criterion needs to be adjusted so that the nitrogen as measured in the discharge corresponds to the form used in the TWF. To do this, we need to convert the ammonia-as-nitrogen water quality criterion to an ammonia-as- NH_3 basis by multiplying by the ratio of the molecular weights, i.e. $4,150 \times (17/14) = 5,039$. Therefore, there will be slight differences between the TWFs for ammonia depending on whether the discharges are reported as nitrogen or as un-ionized ammonia.

6.4.2.2 Nitrate

None of the ecotoxicological studies for nitrate as CAS 14797558 pass the ASTER filter. In fact, the ASTER report lists only one study for freshwater aquatic animals.⁷ EPA reviewed the citation (Lewis et al., 1995). They report no statistically significant response at nitrate concentrations up to 75,000 $\mu\text{g/L}$.

⁶The water quality criterion is under review but the 1999 Update is the most recent available published criterion.

⁷Another study is listed in EPA's ECOTOX database. It dates to 1973, and its absence from the ASTER listing indicates that it might not be the best information source for a TWF.

Accordingly, we propose to use an acute freshwater criterion of 75,000 µg/L and a chronic freshwater criterion of 7,500 µg/L to reflect the upper range at which no effect was seen.

TRI guidance, however, indicates that releases of water-dissociable nitrate compounds are reported in terms of the nitrate ion (TRI, 2000b). The concentrations in Lewis et al. (1995) are reported as NO₃-N, indicating that the aquatic component of the TWF and the TRI pounds are both in terms of the nitrate ion.

6.4.2.3 Nitrite

A search of the ASTER database for “nitrite CAS 14797650” turned up no ecotoxicological studies. Nitrite is an intermediate product in the nitrogen cycle and its relative instability might indicate that it is inappropriate to scale the nitrate TWF by the relative weights of NO₂ and NO₃ to estimate the toxicity for nitrite. EPA (2005b) notes that nitrite is toxic to aquatic species. At the moment, EPA does not believe it can estimate an aquatic health component of the TWF for nitrite regardless of the form in which it is measured and/or reported.

6.4.2.4 Extrapolation to Other Forms of Nitrogen

For undifferentiated components of the nitrogen cycle, EPA proposes to use the average of the ammonia-as-N and nitrate-as-N values. To place the nitrate aquatic health criterion on a nitrogen basis, we would multiply 7,500 µg/L by the ratio of atomic weights for N/NO₃ (i.e., 0.233). The resulting value is 1,748 µg/L, which, when normalized to copper, provides an aquatic health TWF component of 3.20e-3. This is similar to the value for the much more studied ammonia-as-N of 1.35e-3. The average of the two values is 2.28e-3. EPA proposes that the 2.28e-3 aquatic health component for nitrate/nitrite mixtures be used for all measures that have been converted to nitrogen-equivalents.

TRI has an entry reported as “Nitrogen (as NO₃) Sludge Solid.” It is illogical that a facility would go through the effort to de-water a sludge to produce a solid only to discharge the end product to the water. Unless the engineers have a better understanding of this discharge, EPA assumes that the facility generated a process sludge that they tested for nitrate content and reported the discharge in terms of

pounds of nitrate. Presumably, the Kjeldahl method was not used; otherwise the discharge would have been reported as Kjeldahl nitrogen, either as TKN or nitrogen. APHA et al. (1995) describe other methods for determining nitrates. For this entry, then, we propose to use the original NO_3 basis for the aquatic health criterion, that is, $7.47\text{e-}4$. Because it is a single entry in the discharge data base, whatever value for nitrogen is used will have minuscule effect on the industry rankings.

6.4.2.5 Forms for Which There Is Insufficient Information

As mentioned above, the Kjeldahl methods measure organic nitrogen and ammonia. When a discharge is measured in terms of TKN, EPA knows neither the make-up of the organic material nor the proportion of ammonia. Without this knowledge, EPA cannot estimate a TWF for TKN.⁸

Similarly, EPA cannot estimate a TWF for the entry reported as “Nitrogen, Inorganic Total” because it is not known whether the results are reported as the total mass, the nitrite/nitrate portion, or the nitrogen portion.

6.4.3 Nitrogen TWF Summary

Table 6-6 summarizes the TWFs for various forms of nitrogen. Sodium nitrite has the highest TWF ($3.73\text{e-}1$). As noted above, this value is for rainbow trout, a very sensitive species. The TWFs for components of the organic nitrogen cycle are two or more orders of magnitude lower.

Two observations arise from the review of nitrogen data. First, it is necessary to verify whether discharges of sodium nitrite in TRI are sodium nitrite (for which we have numerous studies in ASTER and a proposed TWF) or an unspecified form of nitrite (for which we either have a much lower TWF or no TWF). Second, TWFs measure toxicity. They do not measure the possible eutrophication impacts of nutrients. An alternative measure for eutrophication effects should be developed for nutrients.

⁸We presume that discharges identified as “Nitrogen, Kjeldahl Total (as N)” were converted to this basis according to the composition of the discharge.

Table 6-6
Proposed TWF Summary for Various Forms of Nitrogen

Chemical	Freshwater Chronic Aquatic Health Criteria (µg/L)	Normalized to Copper (TWF)
Sodium nitrite	1.50e+01	3.73e-01
Ammonia (as N)	4.15e+03	1.35e-03
Ammonia (as NH ₃)	(a)	1.11e-03
Nitrate (as NO ₃)	7.50e+03	7.47e-04
Nitrate (as N)	(a)	3.20e-03
Nitrogen, total (as N) Nitrogen, Kjeldahl total (as N) Nitrogen oxides (as N) Nitrogen, organic total (as N)	(a)	2.28e-03
Nitrogen (as NO ₃) sludge solid	7.50e+03	7.47e-04
Nitrogen, nitrite total (as N) Nitrite nitrogen, dissolved (as N) Nitrogen, nitrite total (as NO ₂)	N/A	N/A

(a) Blank cells for criteria indicate that the normalized values are either averages or involve a conversion based on the form in which the nitrogen is measured.

Source: EPA estimates.

6.5 Drinking Water Contaminants

On February 24, 2005, EPA published its second list of contaminant candidates for drinking water (EPA, 2005a). The list has 9 microbiological contaminants and 42 chemical contaminants or contaminant groups. Of the chemical contaminants, the TWF database needs information for those listed in Table 6-7. That table's third column identifies chemicals for which neither human nor aquatic health data can be found on which to base a criterion. Sections 6.5.1 through 6.5.4 discuss chemicals for which TWFs can be estimated. Section 6.5.5 summarizes the TWFs for the drinking water candidate contaminants.

Table 6-7
Drinking Water Candidate Contaminants Needing TWFs

CHEMICAL	CAS	Information Available
1,1-dichloropropene	563586	No
2,2-dichloropropane	594207	No
Acetochlor	34256821	Yes
Alachlor ESA and other acetanilide pesticide degradation products	N/A	See Section 6.5.1
Bromobenzene	108861	Yes
Organotins	N/A	See Section 6.5.2
Perchlorate	14797730	See Section 6.5.3
RDX	121824	
Triazines and degradation products of triazines	Including, but not limited to, cyanazine 21725-46-2 and atrazine-desethyl 6190-65-4	See Section 6.5.4
DCPA mono-acid degradate	887547	No
DCPA di-acid degradate	2136790	Yes

Source: EPA estimates.

6.5.1 Alachlor ESA and Other Acetanilide Pesticide Degradation Products

The Pesticide Action Network database (2005) identifies four breakdown products for alachlor:

- 2,6 diethylaniline, CAS 579-66-8
- 2-hydroxy alachlor (no CAS number)
- Alachlor ethanesulfonic acid (ESA) (no CAS number)
- Alachlor oxanilic acid (no CAS number)

EPA searched Chemfinder for CAS numbers for the last three chemicals and did not find any. ASTER searches need to have the CAS number or chemical formula in SMILES format, so EPA could not request a search on the last three chemicals. ASTER contained data for diethylaniline, 2,6 (CAS 579-66-8). EPA named the entry for this group of chemicals by the name of the chemical for which it has data (i.e.,

diethylaniline, 2,6 CAS 579-66-8). EPA updated the entry for alachlor (CAS 15972-60-8) with the ASTER data for that chemical.

6.5.2 Organotins

Organotins are compounds containing at least one bond between tin and carbon. EPA (1999b) lists cyhexatin, fenbutatin oxide, and fentin hydroxide (TPTH) under organotins. All three examples are triorganotin compounds, meaning that each contains three tin-carbon bonds. From this, we assume that the drinking water list means triorganotin compounds when it simply lists “organotins.” Triorganotin compounds are used as biocides and pesticides while mono- and diorganotin compounds tend to be used in stabilizer, catalyst, and glass-coating applications (Batt, 2005). EPA (2003) notes that the toxicity to aquatic organisms generally increases as the number of organic components increases from one to three and decreases with the addition of a fourth organic component. That is, the triorganotin compounds are more toxic.

However, EPA (1999b) does not list tributyltin (TBT, CAS 688-73-3) or tributyltin oxide (TBTO, CAS 56-35-9) among the organotins even though they have been widely used and studied. EPA published ambient aquatic life water quality criteria in 2003 for tributyltin as TBT (EPA, 2003). EPA adjusted all the chemicals tested to TBT. Because the newly published study incorporates many organotins in the estimation of water quality criteria for organic health for TBT, EPA proposes to use the tributyltin TWF for the organotins TWF. Tributyltin is already in the TWF database but will be updated.

6.5.3 Perchlorate

EPA recently published an IRIS profile for perchlorate and perchlorate salts (IRIS, 2005c). EPA requested ASTER data for perchlorate as well as four perchlorate salts (ammonium, lithium, potassium, and sodium); ASTER has data for potassium and sodium perchlorate. Chronic data exist for potassium perchlorate for freshwater sea lampreys: hormonal effects were seen at 100,000 µg/L during a 122-day exposure. An older study for the effects of 96-hour exposure of trout to sodium perchlorate showed 100 percent mortality at 3,000,000 µg/L. Neither study passed the ASTER filter on quality. EPA used the data for potassium perchlorate for the aquatic health criteria for perchlorate.

6.5.4 Triazines and Degradation Products

EPA has traditionally used the term “triazines” to refer to atrazine, simazine, and cyanazine. EPA (2002c) identifies desisopropyl s-atrazine (DIA), desethyl s-atrazine (DEA) and diaminochlorotriazine (DACT) as metabolites with a common mechanism. It is presumed that the TWF for triazines and degradation products should reflect available information for these six chemicals. Unfortunately, no human or aquatic health data could be located for the three metabolites. Table 6-8 summarizes the human health and aquatic life criteria for atrazine, simazine, and cyanazine. It is suggested that EPA use the geometric mean of the three values for a triazine TWF. The human health component will be calculated on the basis of the cancer slope factor (q1*).

Table 6-8
Human and Aquatic Health Data for Triazines and Degradation Products

Chemical	Human Health		BCF	Aquatic-Fresh		Aquatic-Salt	
	RfD	q1*		Chronic	Acute	Chronic	Acute
Atrazine	3.50e-02	2.20e-01	31	65	6,700		2,600
Simazine	5.00e-03	1.20e-01	18	1,000	124,875		
Cyanazine	2.00e-03	8.40e-01	4.0	3.5			
Geometric Mean (µg/L)	7.00e-03	2.80e-01	13	61	29,000		2,600
Toxic Weighting Factor							
Component Value	7.95e+02	1.99e+01		0.0918	0.0002		0.0022

Source: ASTER, 2005.

6.5.5 Summary

Table 6-9 lists the proposed TWFs for drinking water contaminants. The worksheets are located in Appendix A-28 through A-43.

Table 6-9
Drinking Water Candidate Contaminants Needing TWFs

Chemical	CAS	Proposed TWF
1,1-dichloropropene	563586	0
2,2-dichloropropane	594207	0
Acetochlor	34256821	1.48e-2
Alachlor (update)	15972608	1.52e+0
2,6-diethylaniline (alachlor degradation product)	579668	5.38e-4
Bromobenzene	108861	7.58e-3
Tributyltin (organotins)	688733	7.78e+1
Perchlorate	14797730	2.00e-3
RDX	121824	4.15e-3
Triazines	N/A	2.46e+0
Atrazine	1912249	1.04e+0
Simazine	122349	3.08e-1
Cyanazine	21725462	4.70e+0
DCPA mono-acid degradate	887547	0
DCPA di-acid degradate	2136790	4.10e-4

Source: EPA estimates.

6.6 NICOTINE

6.6.1 Human Health

Nicotine is a poison with a lethal dose in adults of 0.5 to 1.0 mg/kg of body weight, or a total dose of 30 to 60 mg (Boulton et al., 2003). In 2003, Michigan officials arrested a person for contaminating 200 pounds of ground beef with Black Leaf 40—a pesticide containing 40 percent nicotine—and thereby affecting about 100 people. EPA canceled its product registration of Black Leaf in 1992 because of its toxicity (Boulton et al., 2003). In 2002, EPA revoked Federal Food, Drug, and Cosmetic Act tolerances for residues of nicotine-containing compounds on agricultural products except cucumber, lettuce, and tomato (EPA, 2002d). EPA plans to publish a Reregistration Eligibility Decision (RED) on nicotine in fiscal year 2008. In the Notice, nicotine is listed as a pesticide with no associated tolerance (EPA, 2004).

Dermal exposure to nicotine can result in “green tobacco sickness” (GTS) marked by nausea, vomiting, weakness, dizziness, and sometimes fluctuations in blood pressure or heart rate. During a particularly wet harvesting season in 1992, Kentucky reported an outbreak of 27 cases of GTS severe enough that emergency room treatment was sought. A review of hospital records identified 55 possible cases of GTS in Kansas between May and October of 1992. Dew from tobacco leaves often saturated workers’ clothing within minutes of beginning field work (Boylan et al., 1993). Because it is connected to factory workers, this exposure route lies more in OSHA’s purview than EPA’s, but it is indicative of the toxicity of nicotine.

However, EPA checked its traditional sources⁹ for a RfD or a cancer slope and did not identify either for nicotine. In other words, the TWF for nicotine will be underestimated due to the absence of data for calculating a human health component.

⁹IRIS; April 2005 Region 3 Risk Based Concentration/HEAST tables; ATSDR toxicological profiles; California Environmental Protection Agency, Proposition 65 list (where nicotine was not placed on the candidate list in a March 2004 carcinogenicity evaluation); NIH/NIEHS/Center for Evaluation of Risks to Human Reproduction (which deferred a review in 2000 for chemicals with higher priorities); and Toxicity and Chemical Specific Factors Data Base, Risk Assessment Information System, located at <http://risk.lsd.ornl.gov>.

6.6.2 Aquatic Health

A search of the ASTER database identified one study for nicotine that passed the ASTER filter (Passino-Reader et al., 1995). The tested species is freshwater rainbow trout and the concentration levels are:

- 60-day LC₅₀: 5,000 µg/L
- 60-day LOEC: 4,200 µg/L
- 60-day NOEC: 2,900 µg/L

We calculate a maximum allowable toxicant concentration (MACT) by taking the geometric mean of the NOEC and LOEC values, i.e., $\sqrt[2]{4200 \times 2900}$ or 3,490. In accordance with Zipf (2003) the MACT is the preferred value for the aquatic health criterion. Normalizing this to copper, i.e., 5.6/3,490, results in an aquatic health TWF component of **1.6 e-3**. The worksheet for nicotine is located in Appendix A-44.

6.7 REFERENCES

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ATTACHMENT A
TWF DATA WORKSHEETS

Pollutant: Hydrogen Fluoride			CAS: 7664393
Variable	Units	Value	Source
Human Health			
q1*	mg/kg-day		Value is for Fluoride. ATSDR, 2003. Toxicological Profile for Fluorides, Hydrogen Fluoride, and Fluorine. September. IRIS, 2004; 0.06 mg/kg-day for fluorine (soluble fluoride, CAS 7782414) RfD verification date, 1985.
Carcinogen flag	Y/N	N	
RfD	mg/kg-day	0.05	
Code	NOAEL		
BCF	L/kg		
BAF			
RSC			
Aquatic—Freshwater—Chronic			
AWQC	µg/L		no hits in ASTER or ECOTOX
Code			
Species			
Aquatic—Freshwater—Acute			
AWQC	µg/L		
Code			
Species			
Aquatic—Saltwater—Chronic			
AWQC	µg/L		
Code			
Species			
Aquatic—Saltwater—Acute			
AWQC	µg/L		
Code			
Species			

Pollutant: Chlorine Dioxide			CAS: 10049044
Variable	Units	Value	Source
Human Health			
q1*	mg/kg-day		IRIS, 2004; Carcinogen assessment consensus date, 2000. Class: D not classifiable because of inadequate data.
Carcinogen flag	Y/N	N	
RfD	mg/kg-day	0.03	IRIS, 2004; RfD consensus date, 2000.
Code	NOAEL with uncertainty factor		
BCF	L/kg		
BAF			
RSC			
Aquatic—Freshwater—Chronic			
AWQC	µg/L	35	ASTER, 2004; Ref. 17656. Matisoff, G, G Brooks, and BI Borland. Toxicity of Chlorine Dioxide to Adult Zebra Mussels. J. Am. Water Works Assoc. 88:93-106. 1996.
Code	Estimated From Acute Value Using Acute-Chronic Ratio of 10; See U.S. EPA. Technical Support Document for Water Quality-based Toxics Control. EPA 505/2-90-001. March 1991.		
Species	Zebra Mussel		
Aquatic—Freshwater—Acute			
AWQC	µg/L	350	ASTER, 2004; Ref. 17656. Matisoff, G, G Brooks, and BI Borland. Toxicity of Chlorine Dioxide to Adult Zebra Mussels. J. Am. Water Works Assoc. 88:93-106. 1996.
Code	lowest reported 96-hr LC ₅₀		
Species	Zebra Mussel		
Aquatic—Saltwater—Chronic			
AWQC	µg/L	50,000	ASTER, 2004; Ref. 906. Portmann, JE and KW Wilson. The Toxicity of 140 Substances to the Brown Shrimp and Other Marine Animals. Shellfish Information Leaflet No. 22 (2 nd ed.) Ministry of Agric. Fish. Food, Fish. Lab. Burnham-on-Crouch, Essex and Fish Exp. Station, Conway, North Wales, 12p. 1971.
Code	Estimated From Acute Value Using Acute-Chronic Ratio of 10; See U.S. EPA. Technical Support Document for Water Quality-based Toxics Control. EPA 505/2-90-001. March 1991.		
Species	Green Crab		
Aquatic—Saltwater—Acute			
AWQC	µg/L	500,000	ASTER, 2004; Ref. 906. Portmann, JE and KW Wilson. The Toxicity of 140 Substances to the Brown Shrimp and Other Marine Animals. Shellfish Information Leaflet No. 22 (2 nd ed.) Ministry of Agric. Fish. Food, Fish. Lab. Burnham-on-Crouch, Essex and Fish Exp. Station, Conway, North Wales, 12p. 1971.
Code	lowest reported 48-hr LC ₅₀		
Species	Green Crab		

Pollutant: 1, 3-Phenylenediamine			CAS: 108452
Variable	Units	Value	Source
Human Health			
q1*	mg/kg-day		IRIS, 2004; no data.
Carcinogen flag	Y/N	N	
RfD	mg/kg-day	6e-3	IRIS, 2004; RfD verification date, 1986.
Code	NOEL with uncertainty factor		
BCF	L/kg	1	ASTER, 2004; QSAR estimate.
BAF			
RSC			
Aquatic—Freshwater—Chronic			
AWQC	µg/L	38,009	ASTER, 2004; QSAR estimate.
Code	Estimated From Acute Value Using Acute-Chronic Ratio of 10; See U.S. EPA. Technical Support Document for Water Quality-based Toxics Control. EPA 505/2-90-001. March 1991.		
Species	Channel Catfish		
Aquatic—Freshwater—Acute			
AWQC	µg/L	380,089	ASTER, 2004; QSAR estimate.
Code	lowest reported 96-hr LC ₅₀		
Species	Channel Catfish		
Aquatic—Saltwater—Chronic			
AWQC	µg/L		
Code			
Species			
Aquatic—Saltwater—Acute			
AWQC	µg/L		
Code			
Species			

Pollutant: Benzo(a)pyrene			CAS: 50328
Variable	Units	Value	Source
Human Health			
q1*	mg/kg-day	7.3	EPA. 2002. National Recommended Water Quality Criteria: 2002 Human Health Calculation Matrix. EPA 822-R-02-012.
Carcinogen flag	Y/N	Y	
RfD	mg/kg-day		
Code			EPA. 2002. National Recommended Water Quality Criteria: 2002 Human Health Calculation Matrix. EPA 822-R-02-012.
BCF	L/kg	30	
BAF			
RSC			
Aquatic—Freshwater—Chronic			
AWQC	µg/L	0.08	ASTER 2004; Ref. 10412. Hannah, JB, JE hose, ML Landolt, BS Miller, SP Felton, WT Iwaoka. Benzo(a)pyrene-induced Morphological and Developmental Abnormalities in Rainbow Trout. Arch. Environ. Contam. Toxicol. 11(6):727-734. 1982.
Code	lowest reported growth effect		
Species	Rainbow Trout		
Aquatic—Freshwater—Acute			
AWQC	µg/L	5	ASTER 2004; Ref. 15337. Trucco, RG, FR Englehart, B Stacey. Toxicity, Accumulation and Clearance of Aromatic Hydrocarbons in Daphnia pulex. Environ. Pollut. Ser. A Ecol. Biol. 31(3):191-202. 1983,
Code	lowest reported 96-hr LC ₅₀		
Species	Water Flea		
Aquatic—Saltwater—Chronic			
AWQC	µg/L	100	ASTER 2004; Ref. 5053. Rossi, SS and JM Neff. Toxicity of Polynuclear Aromatic Hydrocarbons to the Polychaete Neanthes arenaceodentata, Mar. Pollut. Bull. 9(8):220-223. 1978.
Code	Estimated From Acute Value Using Acute-Chronic Ratio of 10; See U.S. EPA. Technical Support Document for Water Quality-based Toxics Control. EPA 505/2-90-001. March 1991.		
Species	Polychaete Worm		
Aquatic—Saltwater—Acute			
AWQC	µg/L	1,000	ASTER 2004; Ref. 5053. Rossi, SS and JM Neff. Toxicity of Polynuclear Aromatic Hydrocarbons to the Polychaete Neanthes arenaceodentata, Mar. Pollut. Bull. 9(8):220-223. 1978.
Code	lowest reported 96-hr LC ₅₀		
Species	Polychaete Worm		

Pollutant: Aniline			CAS: 62533
Variable	Units	Value	Source
Human Health			
q1*	mg/kg-day	5.7e-3	IRIS, 2004; Carginogenicity assessment verifications date, 1987. Class: B2 probable human carcinogen
Carcinogen flag	Y/N	Y	
RfD	mg/kg-day		
Code			
BCF	L/kg	7	ASTER, 2004; Arithmetic average of seven studies.
BAF			
RSC			
Aquatic—Freshwater—Chronic			
AWQC	µg/L	4,400	ASTER, 2004; Ref. 538. Birge, W.J., JA Black, JE Hudson, and DM Bruser. Embryo-Larval Toxicity Tests with Organic Compounds. In LL Marking and RA Kimerle (eds.) Aquatic Toxicology and Hazard Assessment, 2 nd Symposium, ASTM STP 667, Philadelphia, PA;131-147. 1979
Code	lowest LC ₅₀		
Species	Largemouth Bass		
Aquatic—Freshwater—Acute			
AWQC	µg/L	68,630	ASTER, 2004; Ref. 3910. Marchinie, S, ML Tosato, TJ Norberg-King, DE Hammermeister, and MD Holund. Lethal and Sublethal Toxicity of Benzene Derivatives to the Fathead Minnow, Using a Short-Term Test. Environ. Toxicol. Chem 11(2):187-195. 1992.
Code	lowest 96-hr LC ₅₀		
Species	Fathead Minnow		
Aquatic—Saltwater—Chronic			
AWQC	µg/L	2,940	ASTER, 2004; Ref. 5810. McLeese, DW, V Zitko, and MR Peterson. Structure-Lethality Relationships for Phenols, Anilines, and Other Aromatic Compounds in Shrimp and Clams. Chemosphere 8(2):53-57. 1979.
Code	Estimated From Acute Value Using Acute-Chronic Ratio of 10; See U.S. EPA. Technical Support Document for Water Quality-based Toxics Control. EPA 505/2-90-001. March 1991.		
Species	Bay Shrimp/Sand Shrimp		
Aquatic—Saltwater—Acute			
AWQC	µg/L	29,400	ASTER, 2004; Ref. 5810. McLeese, DW, V Zitko, and MR Peterson. Structure-Lethality Relationships for Phenols, Anilines, and Other Aromatic Compounds in Shrimp and Clams. Chemosphere 8(2):53-57. 1979.
Code	lowest 96-hr LC ₅₀		
Species	Bay Shrimp/Sand Shrimp		

Pollutant: Vanadium			CAS: 7440622
Variable	Units	Value	Source
Human Health			
q1*	mg/kg-day		EPA-NCEA provisional value from Region III, Risk-Based Concentration Table, dated 10/8/2004.
Carcinogen flag	Y/N	N	
RfD	mg/kg-day	1e-3	
Code			
BCF	L/kg		
BAF			
RSC			
Aquatic—Freshwater—Chronic			
AWQC	µg/L	160	ASTER, 2004; Ref. 4943. Birge, JW, JA Black, and AG Westerman. Evaluation of Aquatic Pollutants Using Fish and Amphibian Eggs as Bioassay Organisms. In SW Nielsen, G. Migaki, and DG Scarpelli (Eds.) Symp. Animals Monitors Environ. Pollut. 1977, Storrs, CT 12:108-118. 1979
Code	lowest LC ₅₀		
Species	Rainbow Trout		
Aquatic—Freshwater—Acute			
AWQC	µg/L		
Code			
Species			
Aquatic—Saltwater—Chronic			
AWQC	µg/L	5	ASTER, 2004; Ref. 6761. Ballester, A and J Castellvi. Contribution to the Study of V and Ni Uptake in Marine Organisms (Contribucion al Estudio de la Biocenetica de V y Ni en Organismos Marinos). Invest, Pesq. 43(2):49-478 (Spanish, English abstract).
Code	Estimated From Acute Value Using Acute-Chronic Ratio of 10; See U.S. EPA. Technical Support Document for Water Quality-based Toxics Control. EPA 505/2-90-001. March 1991.		
Species	Common bay mussel		
Aquatic—Saltwater—Acute			
AWQC	µg/L	50	ASTER, 2004; Ref. 6761. Ballester, A and J Castellvi. Contribution to the Study of V and Ni Uptake in Marine Organisms (Contribucion al Estudio de la Biocenetica de V y Ni en Organismos Marinos). Invest, Pesq. 43(2):49-478 (Spanish, English abstract).
Code	lowest reported residue effects		
Species	Common bay mussel		

Pollutant: Mercury			CAS: 7439976
Variable	Units	Value	Source
Human Health			
q1*	mg/kg-day		IRIS, 2004: Carcinogenicity Assessment Verification date, 1994. Class: D - not classifiable as to human carcinogenicity (inadequate data).
Carcinogen flag	Y/N	N	
RfD	mg/kg-day	1.00e-4	IRIS, 2004, not available. EPA. 2002. National Recommended Water Quality Criteria: 2002 - Human Health Criteria Calculation Matrix. EPA-822-R-02-012. November. Based on 1997 IRIS value.
Code			
BCF	L/kg	7342.6	EPA. 2002. National Recommended Water Quality Criteria: 2002 - Human Health Criteria Calculation Matrix. EPA-822-R-02-012. November
BAF			
RSC		1	EPA. 2002. National Recommended Water Quality Criteria: 2002 - Human Health Criteria Calculation Matrix. EPA-822-R-02-012. November. 1998 Value calculated with 1980 methodology.
FI		18.7	EPA. 2002. National Recommended Water Quality Criteria: 2002 - Human Health Criteria Calculation Matrix. EPA-822-R-02-012. November
Aquatic—Freshwater—Chronic			
AWQC	µg/L	0.77	EPA. 2002. National Recommended Water Quality Criteria: 2002. EPA-822-R-02-047. November
Code			
Species			
Aquatic—Freshwater—Acute			
AWQC	µg/L	1.4	EPA. 2002. National Recommended Water Quality Criteria: 2002. EPA-822-R-02-047. November
Code			
Species			
Aquatic—Saltwater—Chronic			
AWQC	µg/L	0.94	EPA. 2002. National Recommended Water Quality Criteria: 2002. EPA-822-R-02-047. November
Code			
Species			
Aquatic—Saltwater—Acute			
AWQC	µg/L	1.8	EPA. 2002. National Recommended Water Quality Criteria: 2002. EPA-822-R-02-047. November
Code			
Species			

Pollutant: Methylmercury			CAS: 22967926
Variable	Units	Value	Source
Human Health			
q1*	mg/kg-day		IRIS, 2004; Carcinogenicity Assessment date 1995. Classification = C; possible human carcinogen but systemic affects would likely been seen at exposures lower than those required for tumor formation.
Carcinogen flag	Y/N	Y	
RfD	mg/kg-day	1.00e-4	IRIS, 2004; Oral RfD consensus date 2001.
Code	BMDL50 benchmark dose, lower limit 95%		
BCF			
BAF		1,225,029	Methylmercury Water Quality Criteria. Jan 8, 2001. 66 FR 1344-1359. Calculated as weighted average of fish intake and BAF for fish intake of 17.5 grams/day. See memo to Lynn Zipf, EPA, dated 14 December 2004.
RSC		73%	Methylmercury Water Quality Criteria. Jan 8, 2001. 66 FR 1344-1359. RSC presented as an amount to subtract. Converted to percentage. See memo to Lynn Zipf, EPA, dated 14 December 2004.
Aquatic—Freshwater—Chronic			
AWQC	µg/L		
Code			
Species			
Aquatic—Freshwater—Acute			
AWQC	µg/L		
Code			
Species			
Aquatic—Saltwater—Chronic			
AWQC	µg/L		
Code			
Species			
Aquatic—Saltwater—Acute			
AWQC	µg/L		
Code			
Species			

Pollutant: Benzo(a)anthracene			CAS: 56553
Variable	Units	Value	Source
Human Health			
q1*	mg/kg-day	7.3	Value for benzo(b)fluoranthene (CAS 205992). USEPA. 2002. National Recommended Water Quality Criteria: 2002 Human Health Calculation Matrix. EPA 822-R-02-012.
Carcinogen flag	Y/N	Y	
RfD	mg/kg-day		
Code			
BCF	L/kg	30	Value for benzo(b)fluoranthene (CAS 205992). USEPA. 2002. National Recommended Water Quality Criteria: 2002 Human Health Calculation Matrix. EPA 822-R-02-012.
BAF			
RSC			
Aquatic—Freshwater—Chronic			
AWQC	µg/L	160	ASTER. 2004. QSAR est., Ref. 15823. Veith, GD, DJ Call, and LT Brooke. Structural-Toxicity Relationships for the Fathead Minnow, Pimephales promelas: Narcotic Industrial Chemicals. Can J. Fish. Aquat. Sci. 40(6):743-748. 1983.
Code	Estimated From Acute Value Using Acute-Chronic Ratio of 10; USEPA. Technical Support Document for Water Quality-based Toxics Control. EPA 505/2-90-001. March 1991.		
Species	Fathead Minnow		
Aquatic—Freshwater—Acute			
AWQC	µg/L	1599	ASTER. 2004. QSAR est., Ref. 15823. Veith, GD, DJ Call, and LT Brooke. Structural-Toxicity Relationships for the Fathead Minnow, Pimephales promelas: Narcotic Industrial Chemicals. Can J. Fish. Aquat. Sci. 40(6):743-748. 1983.
Code	96-hr LC ₅₀		
Species	Fathead Minnow		
Aquatic—Saltwater—Chronic			
AWQC	µg/L	7.5	ASTER. 2004. Ref. 3511. A.E. McElroy. Polycyclic Aromatic Hydrocarbon Metabolism in the Polychaete Nereis virens. Aquat. Toxicol. 18(1):35-50. 1990.
Code	Estimated From Acute Value Using Acute-Chronic Ratio of 10; USEPA. Technical Support Document for Water Quality-based Toxics Control. EPA 505/2-90-001. March 1991.		
Species	Polychaete worm		
Aquatic—Saltwater—Acute			
AWQC	µg/L	75	ASTER. 2004. Ref. 3511. A.E. McElroy. Polycyclic Aromatic Hydrocarbon Metabolism in the Polychaete Nereis virens. Aquat. Toxicol. 18(1):35-50. 1990.
Code	lowest reported biological effect		
Species	Polychaete worm		

Pollutant: Benzo(a)phenanthrene (Chrysene)			CAS: 218019
Variable	Units	Value	Source
Human Health			
q1*	mg/kg-day	7.3	Value for benzo(b)fluoranthene (CAS 205992). USEPA. 2002. National Recommended Water Quality Criteria: 2002 Human Health Calculation Matrix. EPA 822-R-02-012.
Carcinogen flag	Y/N	Y	
RfD	mg/kg-day		
Code			
BCF	L/kg	30	Value for benzo(b)fluoranthene (CAS 205992). USEPA. 2002. National Recommended Water Quality Criteria: 2002 Human Health Calculation Matrix. EPA 822-R-02-012.
BAF			
RSC			
Aquatic—Freshwater—Chronic			
AWQC	µg/L	160	ASTER. 2004. QSAR est., Ref. 15823. Veith, GD, DJ Call, and LT Brooke. Structural-Toxicity Relationships for the Fathead Minnow, Pimephales promelas: Narcotic Industrial Chemicals. Can J. Fish. Aquat. Sci. 40(6):743-748. 1983.
Code	Estimated From Acute Value Using Acute-Chronic Ratio of 10; USEPA. Technical Support Document for Water Quality-based Toxics Control. EPA 505/2-90-001. March 1991.		
Species	Fathead Minnow		
Aquatic—Freshwater—Acute			
AWQC	µg/L	1599	ASTER. 2004. QSAR est., Ref. 15823. Veith, GD, DJ Call, and LT Brooke. Structural-Toxicity Relationships for the Fathead Minnow, Pimephales promelas: Narcotic Industrial Chemicals. Can J. Fish. Aquat. Sci. 40(6):743-748. 1983.
Code	96-hr LC ₅₀		
Species	Fathead Minnow		
Aquatic—Saltwater—Chronic			
AWQC	µg/L		ASTER. 2004. No data.
Code			
Species			
Aquatic—Saltwater—Acute			
AWQC	µg/L		ASTER. 2004. No data.
Code			
Species			

Pollutant: Benzo(b)fluoranthene			CAS: 205992
Variable	Units	Value	Source
Human Health			
q1*	mg/kg-day	7.3	USEPA. 2002. National Recommended Water Quality Criteria: 2002 Human Health Calculation Matrix. EPA 822-R-02-012.
Carcinogen flag	Y/N	Y	
RfD	mg/kg-day		
Code			
BCF	L/kg	30	USEPA. 2002. National Recommended Water Quality Criteria: 2002 Human Health Calculation Matrix. EPA 822-R-02-012.
BAF			
RSC			
Aquatic—Freshwater—Chronic			
AWQC	µg/L		ASTER. 2004. No data.
Code			
Species			
Aquatic—Freshwater—Acute			
AWQC	µg/L		ASTER. 2004. No data.
Code			
Species			
Aquatic—Saltwater—Chronic			
AWQC	µg/L		ASTER. 2004. No data.
Code			
Species			
Aquatic—Saltwater—Acute			
AWQC	µg/L		ASTER. 2004. No data.
Code			
Species			

Pollutant: Benzo(k)fluoranthene			CAS: 207089
Variable	Units	Value	Source
Human Health			
q1*	mg/kg-day	7.3	Value for benzo(b)fluoranthene (CAS 205992). USEPA. 2002. National Recommended Water Quality Criteria: 2002 Human Health Calculation Matrix. EPA 822-R-02-012.
Carcinogen flag	Y/N	Y	
RfD	mg/kg-day		
Code			Value for benzo(b)fluoranthene (CAS 205992). USEPA. 2002. National Recommended Water Quality Criteria: 2002 Human Health Calculation Matrix. EPA 822-R-02-012.
BCF	L/kg	30	
BAF			
RSC			
Aquatic—Freshwater—Chronic			
AWQC	µg/L		ASTER. 2004. No data.
Code			
Species			
Aquatic—Freshwater—Acute			
AWQC	µg/L		ASTER. 2004. No data.
Code			
Species			
Aquatic—Saltwater—Chronic			
AWQC	µg/L		ASTER. 2004. No data.
Code			
Species			
Aquatic—Saltwater—Acute			
AWQC	µg/L		ASTER. 2004. No data.
Code			
Species			

Pollutant: Benzo(j,k)fluoranthene (fluoranthene)			CAS: 206440
Variable	Units	Value	Source
Human Health			
q1*	mg/kg-day		
Carcinogen flag	Y/N	N	
RfD	mg/kg-day	0.04	USEPA. 2002. National Recommended Water Quality Criteria: 2002 Human Health Calculation Matrix. EPA 822-R-02-012.
Code			
BCF	L/kg	1150	USEPA. 2002. National Recommended Water Quality Criteria: 2002 Human Health Calculation Matrix. EPA 822-R-02-012.
BAF			
RSC			
Aquatic—Freshwater—Chronic			
AWQC	µg/L	4.5	ASTER. 2004. Ref. 3590. Oris, JT, RW Winner, and MV Moore. A Four-Day Survival and reproduction Toxicity Test for Ceriodaphnia dubia. Environ. Toxicol. Chem. 10(2): 217-224. 1991.
Code	Estimated From Acute Value Using Acute-Chronic Ratio of 10; USEPA. Technical Support Document for Water Quality-based Toxics Control. EPA 505/2-90-001. March 1991.		
Species	Water flea		
Aquatic—Freshwater—Acute			
AWQC	µg/L	45	ASTER. 2004. Ref. 3590. Oris, JT, RW Winner, and MV Moore. A Four-Day Survival and reproduction Toxicity Test for Ceriodaphnia dubia. Environ. Toxicol. Chem. 10(2): 217-224. 1991.
Code	lowest 48-hr LC ₅₀		
Species	Water flea		
Aquatic—Saltwater—Chronic			
AWQC	µg/L		ASTER. 2004. No data.
Code			
Species			
Aquatic—Saltwater—Acute			
AWQC	µg/L		ASTER. 2004. No data.
Code			
Species			

Pollutant: Dibenzo(a,h)anthracene			CAS: 53703
Variable	Units	Value	Source
Human Health			
q1*	mg/kg-day	7.3	Value for benzo(b)fluoranthene (CAS 205992). USEPA. 2002. National Recommended Water Quality Criteria: 2002 Human Health Calculation Matrix. EPA 822-R-02-012.
Carcinogen flag	Y/N	Y	
RfD	mg/kg-day		
Code			
BCF	L/kg	30	Value for benzo(b)fluoranthene (CAS 205992). USEPA. 2002. National Recommended Water Quality Criteria: 2002 Human Health Calculation Matrix. EPA 822-R-02-012.
BAF			
RSC			
Aquatic—Freshwater—Chronic			
AWQC	µg/L	50	ASTER. 2004. Ref. 17714. Wernersson, AS and G Dave. Phototoxicity Identification by Solid Phase Extraction and Photoinduced Toxicity to Daphnia magna. Arch. Environ. Contam. Toxicol. 32(3):268-273. 1997.
Code	Estimated From Acute Value Using Acute-Chronic Ratio of 10; USEPA. Technical Support Document for Water Quality-based Toxics Control. EPA 505/2-90-001. March 1991.		
Species	Water Flea		
Aquatic—Freshwater—Acute			
AWQC	µg/L	496	ASTER. 2004. Ref. 17714. Wernersson, AS and G Dave. Phototoxicity Identification by Solid Phase Extraction and Photoinduced Toxicity to Daphnia magna. Arch. Environ. Contam. Toxicol. 32(3):268-273. 1997.
Code	lowest EC50		
Species	Water Flea		
Aquatic—Saltwater—Chronic			
AWQC	µg/L		ASTER. 2004. No data.
Code			
Species			
Aquatic—Saltwater—Acute			
AWQC	µg/L		ASTER. 2004. No data.
Code			
Species			

Pollutant: Indeno(1,2,3-cd)pyrene			CAS:193395
Variable	Units	Value	Source
Human Health			
q1*	mg/kg-day	7.3	Value for benzo(b)fluoranthene (CAS 205992). USEPA. 2002. National Recommended Water Quality Criteria: 2002 Human Health Calculation Matrix. EPA 822-R-02-012.
Carcinogen flag	Y/N	Y	
RfD	mg/kg-day		
Code			Value for benzo(b)fluoranthene (CAS 205992). USEPA. 2002. National Recommended Water Quality Criteria: 2002 Human Health Calculation Matrix. EPA 822-R-02-012.
BCF	L/kg	30	
BAF			
RSC			
Aquatic—Freshwater—Chronic			
AWQC	µg/L		ASTER. 2004. No data.
Code			
Species			
Aquatic—Freshwater—Acute			
AWQC	µg/L		ASTER. 2004. No data.
Code			
Species			
Aquatic—Saltwater—Chronic			
AWQC	µg/L		ASTER. 2004. No data.
Code			
Species			
Aquatic—Saltwater—Acute			
AWQC	µg/L		ASTER. 2004. No data.
Code			
Species			

Pollutant: Benzo(j)fluoranthene			CAS: 205823
Variable	Units	Value	Source
Human Health			
q1*	mg/kg-day		No data (IRIS, USEPA Region RBC Table, ATSDR toxicological profiles, USEPA 2000, USEPA 1995)
Carcinogen flag	Y/N		
RfD	mg/kg-day		
Code			
BCF	L/kg		
BAF			
RSC			
Aquatic—Freshwater—Chronic			
AWQC	µg/L		ASTER. 2004. No data.
Code			
Species			
Aquatic—Freshwater—Acute			
AWQC	µg/L		ASTER. 2004. No data.
Code			
Species			
Aquatic—Saltwater—Chronic			
AWQC	µg/L		ASTER. 2004. No data.
Code			
Species			
Aquatic—Saltwater—Acute			
AWQC	µg/L		ASTER. 2004. No data.
Code			
Species			

Pollutant: Benzo(r,s,t)pentaphene			CAS: 189559
Variable	Units	Value	Source
Human Health			
q1*	mg/kg-day		No data (IRIS, USEPA Region RBC Table, ATSDR toxicological profiles, USEPA 2000, USEPA 1995)
Carcinogen flag	Y/N		
RfD	mg/kg-day		
Code			
BCF	L/kg		
BAF			
RSC			
Aquatic—Freshwater—Chronic			
AWQC	µg/L		ASTER. 2004. No animal data.
Code			
Species			
Aquatic—Freshwater—Acute			
AWQC	µg/L		ASTER. 2004. No animal data.
Code			
Species			
Aquatic—Saltwater—Chronic			
AWQC	µg/L		ASTER. 2004. No animal data.
Code			
Species			
Aquatic—Saltwater—Acute			
AWQC	µg/L		ASTER. 2004. No animal data.
Code			
Species			

Pollutant: Dibenz(a,h)acridine			CAS: 226368
Variable	Units	Value	Source
Human Health			
q1*	mg/kg-day		No data (IRIS, USEPA Region RBC Table, ATSDR toxicological profiles, USEPA 2000, USEPA 1995)
Carcinogen flag	Y/N		
RfD	mg/kg-day		
Code			
BCF	L/kg		
BAF			
RSC			
Aquatic—Freshwater—Chronic			
AWQC	µg/L		ASTER. 2004. No data.
Code			
Species			
Aquatic—Freshwater—Acute			
AWQC	µg/L		ASTER. 2004. No data.
Code			
Species			
Aquatic—Saltwater—Chronic			
AWQC	µg/L		ASTER. 2004. No data.
Code			
Species			
Aquatic—Saltwater—Acute			
AWQC	µg/L		ASTER. 2004. No data.
Code			
Species			

Pollutant: Dibenz(a,j)acridine			CAS: 224420
Variable	Units	Value	Source
Human Health			
q1*	mg/kg-day		No data (IRIS, USEPA Region RBC Table, ATSDR toxicological profiles, USEPA 2000, USEPA 1995)
Carcinogen flag	Y/N		
RfD	mg/kg-day		
Code			
BCF	L/kg		
BAF			
RSC			
Aquatic—Freshwater—Chronic			
AWQC	µg/L		ASTER. 2004. No animal data.
Code			
Species			
Aquatic—Freshwater—Acute			
AWQC	µg/L		ASTER. 2004. No animal data.
Code			
Species			
Aquatic—Saltwater—Chronic			
AWQC	µg/L		ASTER. 2004. No animal data.
Code			
Species			
Aquatic—Saltwater—Acute			
AWQC	µg/L		ASTER. 2004. No animal data.
Code			
Species			

Pollutant: Dibenzo(a,e)fluoranthene			CAS: 5385751
Variable	Units	Value	Source
Human Health			
q1*	mg/kg-day		No data (IRIS, USEPA Region RBC Table, ATSDR toxicological profiles, USEPA 2000, USEPA 1995)
Carcinogen flag	Y/N		
RfD	mg/kg-day		
Code			
BCF	L/kg		
BAF			
RSC			
Aquatic—Freshwater—Chronic			
AWQC	µg/L		ASTER. 2004. No data.
Code			
Species			
Aquatic—Freshwater—Acute			
AWQC	µg/L		ASTER. 2004. No data.
Code			
Species			
Aquatic—Saltwater—Chronic			
AWQC	µg/L		ASTER. 2004. No data.
Code			
Species			
Aquatic—Saltwater—Acute			
AWQC	µg/L		ASTER. 2004. No data.
Code			
Species			

Pollutant: Dibenzo(a,e)pyrene			CAS: 192654
Variable	Units	Value	Source
Human Health			
q1*	mg/kg-day		No data (IRIS, USEPA Region RBC Table, ATSDR toxicological profiles, USEPA 2000, USEPA 1995)
Carcinogen flag	Y/N		
RfD	mg/kg-day		
Code			
BCF	L/kg		
BAF			
RSC			
Aquatic—Freshwater—Chronic			
AWQC	µg/L		ASTER. 2004. No data.
Code			
Species			
Aquatic—Freshwater—Acute			
AWQC	µg/L		ASTER. 2004. No data.
Code			
Species			
Aquatic—Saltwater—Chronic			
AWQC	µg/L		ASTER. 2004. No data.
Code			
Species			
Aquatic—Saltwater—Acute			
AWQC	µg/L		ASTER. 2004. No data.
Code			
Species			

Pollutant: Dibenzo(a,h)pyrene			CAS: 189640
Variable	Units	Value	Source
Human Health			
q1*	mg/kg-day		No data (IRIS, USEPA Region RBC Table, ATSDR toxicological profiles, USEPA 2000, USEPA 1995)
Carcinogen flag	Y/N		
RfD	mg/kg-day		
Code			
BCF	L/kg		
BAF			
RSC			
Aquatic—Freshwater—Chronic			
AWQC	µg/L		ASTER. 2004. No data.
Code			
Species			
Aquatic—Freshwater—Acute			
AWQC	µg/L		ASTER. 2004. No data.
Code			
Species			
Aquatic—Saltwater—Chronic			
AWQC	µg/L		ASTER. 2004. No data.
Code			
Species			
Aquatic—Saltwater—Acute			
AWQC	µg/L		ASTER. 2004. No data.
Code			
Species			

Pollutant: Dibenzo(a,l)pyrene			CAS: 191300
Variable	Units	Value	Source
Human Health			
q1*	mg/kg-day		No data (IRIS, USEPA Region RBC Table, ATSDR toxicological profiles, USEPA 2000, USEPA 1995)
Carcinogen flag	Y/N		
RfD	mg/kg-day		
Code			
BCF	L/kg		
BAF			
RSC			
Aquatic—Freshwater—Chronic			
AWQC	µg/L		ASTER. 2004. No data.
Code			
Species			
Aquatic—Freshwater—Acute			
AWQC	µg/L		ASTER. 2004. No data.
Code			
Species			
Aquatic—Saltwater—Chronic			
AWQC	µg/L		ASTER. 2004. No data.
Code			
Species			
Aquatic—Saltwater—Acute			
AWQC	µg/L		ASTER. 2004. No data.
Code			
Species			

Pollutant: 7H-dibenzo(c,g)carbazole			CAS: 194592
Variable	Units	Value	Source
Human Health			
q1*	mg/kg-day		No data (IRIS, USEPA Region RBC Table, ATSDR toxicological profiles, USEPA 2000, USEPA 1995)
Carcinogen flag	Y/N		
RfD	mg/kg-day		
Code			
BCF	L/kg		
BAF			
RSC			
Aquatic—Freshwater—Chronic			
AWQC	µg/L	185	ASTER. 2004. QSAR est., Ref. 15823. Veith, GD, DJ Call, and LT Brooke. Structural-Toxicity Relationships for the Fathead Minnow, Pimephales promelas: Narcotic Industrial Chemicals. Can J. Fish. Aquat. Sci. 40(6):743-748. 1983.
Code	Estimated From Acute Value Using Acute-Chronic Ratio of 10; USEPA. Technical Support Document for Water Quality-based Toxics Control. EPA 505/2-90-001. March 1991.		
Species	Fathead Minnow		
Aquatic—Freshwater—Acute			
AWQC	µg/L	1852	ASTER. 2004. QSAR est., Ref. 15823. Veith, GD, DJ Call, and LT Brooke. Structural-Toxicity Relationships for the Fathead Minnow, Pimephales promelas: Narcotic Industrial Chemicals. Can J. Fish. Aquat. Sci. 40(6):743-748. 1983.
Code	96-hr LC ₅₀		
Species	Fathead Minnow		
Aquatic—Saltwater—Chronic			
AWQC	µg/L		ASTER. 2004. No data.
Code			
Species			
Aquatic—Saltwater—Acute			
AWQC	µg/L		ASTER. 2004. Results in fish tissue concentration only.
Code			
Species			

Pollutant: 5-Methylchrysene			CAS: 3697243
Variable	Units	Value	Source
Human Health			
q1*	mg/kg-day		No data (IRIS, USEPA Region RBC Table, ATSDR toxicological profiles, USEPA 2000, USEPA 1995)
Carcinogen flag	Y/N		
RfD	mg/kg-day		
Code			
BCF	L/kg		
BAF			
RSC			
Aquatic—Freshwater—Chronic			
AWQC	µg/L		ASTER. 2004. No data.
Code			
Species			
Aquatic—Freshwater—Acute			
AWQC	µg/L		ASTER. 2004. No data.
Code			
Species			
Aquatic—Saltwater—Chronic			
AWQC	µg/L		ASTER. 2004. No data.
Code			
Species			
Aquatic—Saltwater—Acute			
AWQC	µg/L		ASTER. 2004. No data.
Code			
Species			

Pollutant: 1-Nitropyrene			CAS: 5522430
Variable	Units	Value	Source
Human Health			
q1*	mg/kg-day		No data (IRIS, USEPA Region RBC Table, ATSDR toxicological profiles, USEPA 2000, USEPA 1995)
Carcinogen flag	Y/N		
RfD	mg/kg-day		
Code			
BCF	L/kg		
BAF			
RSC			
Aquatic—Freshwater—Chronic			
AWQC	µg/L	215	ASTER. 2004. QSAR est., Ref. 15823. Veith, GD, DJ Call, and LT Brooke. Structural-Toxicity Relationships for the Fathead Minnow, Pimephales promelas: Narcotic Industrial Chemicals. Can J. Fish. Aquat. Sci. 40(6):743-748. 1983.
Code	Estimated From Acute Value Using Acute-Chronic Ratio of 10; See U.S. EPA. Technical Support Document for Water Quality-based Toxics Control. EPA 505/2-90-001. March 1991.		
Species	Fathead Minnow		
Aquatic—Freshwater—Acute			
AWQC	µg/L	2149	ASTER. 2004. QSAR est., Ref. 15823. Veith, GD, DJ Call, and LT Brooke. Structural-Toxicity Relationships for the Fathead Minnow, Pimephales promelas: Narcotic Industrial Chemicals. Can J. Fish. Aquat. Sci. 40(6):743-748. 1983.
Code	96-hr LC ₅₀		
Species	Fathead Minnow		
Aquatic—Saltwater—Chronic			
AWQC	µg/L		ASTER. 2004. No data.
Code			
Species			
Aquatic—Saltwater—Acute			
AWQC	µg/L		ASTER. 2004. No data.
Code			
Species			

Pollutant: 1,1-dichloropropene			CAS: 563586
Variable	Units	Value	Source
Human Health			
q1*	mg/kg-day		No data (IRIS, USEPA Region RBC Table, ATSDR toxicological profiles, USEPA 2000 [California], USEPA 1995[Great Lakes]).
Carcinogen flag	Y/N		
RfD	mg/kg-day		
Code			
BCF	L/kg		
BAF			
RSC			
Aquatic—Freshwater—Chronic			
AWQC	µg/L		No ASTER data specifically for 1,1, dichloropropene. Reference is to 1980 EPA WQC Document for dichloropropanes and dichloropropenes.
Code			
Species			
Aquatic—Freshwater—Acute			
AWQC	µg/L		
Code			
Species			
Aquatic—Saltwater—Chronic			
AWQC	µg/L		
Code			
Species			
Aquatic—Saltwater—Acute			
AWQC	µg/L		
Code			
Species			

Pollutant: 2,2-dichloropropane			CAS: 594207
Variable	Units	Value	Source
Human Health			
q1*	mg/kg-day		No data (IRIS, USEPA Region RBC Table, ATSDR toxicological profiles, USEPA 2000 [California], USEPA 1995[Great Lakes]).
Carcinogen flag	Y/N		
RfD	mg/kg-day		
Code			
BCF	L/kg		
BAF			
RSC			
Aquatic—Freshwater—Chronic			
AWQC	µg/L		No ASTER data specifically for 2,2 dichloropropane. Reference is to 1980 EPA WQC Document for dichloropropanes and dichloropropenes.
Code			
Species			
Aquatic—Freshwater—Acute			
AWQC	µg/L		
Code			
Species			
Aquatic—Saltwater—Chronic			
AWQC	µg/L		
Code			
Species			
Aquatic—Saltwater—Acute			
AWQC	µg/L		
Code			
Species			

Pollutant: Acetochlor			CAS: 34256821
Variable	Units	Value	Source
Human Health			
q1*	mg/kg-day		IRIS 2005. 1993 revision.
Carcinogen flag	Y/N	N	
RfD	mg/kg-day	2.0e-2	
Code			assumption.
BCF	L/kg	1	
BAF			
RSC			
Aquatic—Freshwater—Chronic			
AWQC	µg/L	38	ASTER. 2005. Ref.: 344. EPA. Office of Pesticide Programs. Environmental Effects Database. 1995.
Code	Estimated From Acute Value Using Acute-Chronic Ratio of 10; See U.S. EPA. Technical Support Document for Water Quality-based Toxics Control. EPA 505/2-90-001. March 1991.		
Species	Rainbow Trout		
Aquatic—Freshwater—Acute			
AWQC	µg/L	380	ASTER. 2005. Ref.: 344. EPA. Office of Pesticide Programs. Environmental Effects Database. 1995. Value cited: 0.38 ppm. ppm = mg/L
Code	96hr LC ₅₀		
Species	Rainbow Trout		
Aquatic—Saltwater—Chronic			
AWQC	µg/L		
Code			
Species			
Aquatic—Saltwater—Acute			
AWQC	µg/L		
Code			
Species			

Pollutant: Alachlor			CAS: 15972-66-8 <i>UPDATE</i>
Variable	Units	Value	Source
Human Health			
q1*	mg/kg-day	8.0e-2	Region 3. Risk Based Concentration Table. 2004. HEAST
Carcinogen flag	Y/N	Y	
RfD	mg/kg-day	1.0e-2	Region 3. Risk Based Concentration Table. 2004. IRIS.
Code			
BCF	L/kg	132	ASTER, 2005. Ref: 7. Veith, G.D. and Kosian. <i>Estimating Bioconcentration Potential from Octanol/Water Partition Coefficients</i> . In D. Mackay et. al. (Eds.), <i>Physical Behavior of PCBs in the Great Lakes</i> . Ann Arbor Sci. Publ., Ann Arbor, MI:269-282. 1983. (Former value 158)
BAF			
RSC			
Aquatic—Freshwater—Chronic			
AWQC	µg/L	140	ASTER, 2005. Ref: 10635. Call,D.J., L.T. Brooke, R.J. Kent, S.H. Poirier, M.L. Knuth, P.J. Shubat, and E.J. Slick. <i>Toxicity, Uptake, and Elimination of the Herbicides Alachlor and Dinoseb in Freshwater Fish</i> . <i>J. Environ. Qual.</i> 13(3):493-498 1984. (Former value 747)
Code	64-day lowest recorded growth effect		
Species	Fathead minnow		
Aquatic—Freshwater—Acute			
AWQC	µg/L	5000	ASTER, 2005. Ref: 15031. Broderius, S.J., M.D. Kahl, and M.D. Hoglund. Use of Joint Toxic Response to Define the Primary Mode of Toxic Action for Diverse Industrial Organic Chemicals. <i>Environ. Toxicol. Chem.</i> 14(9):1591-1605. 1995.
Code	96-hr LC ₅₀		
Species			
Aquatic—Saltwater—Chronic			
AWQC	µg/L		
Code			
Species			
Aquatic—Saltwater—Acute			
AWQC	µg/L		
Code			
Species			

Pollutant: 2, 6-Diethylaniline (Alachlor degradation product)			CAS: 579668
Variable	Units	Value	Source
Human Health			
q1*	mg/kg-day		No data (IRIS, USEPA Region RBC Table, ATSDR toxicological profiles, USEPA 2000 [California], USEPA 1995[Great Lakes]).
Carcinogen flag	Y/N		
RfD	mg/kg-day		
Code			
BCF	L/kg		
BAF			
RSC			
Aquatic—Freshwater—Chronic			
AWQC	µg/L	1042	ASTER. 2005. Ref. 3537. Veith, G.D. and Broderius. Structure-Toxicity Relationships for Industrial Chemicals Causing Type (II) Narcosis Syndrome. In KLE Kaiser (ed.) QSAR in Environmental Toxicology-II, D. Reidel Publ. Co. Dordrecht, Holland:385-391. 1987.
Code	Estimated From Acute Value Using Acute-Chronic Ratio of 10; See U.S. EPA. Technical Support Document for Water Quality-based Toxics Control. EPA 505/2-90-001. March 1991.		
Species	Fathead Minnow		
Aquatic—Freshwater—Acute			
AWQC	µg/L	10417	ASTER. 2005. Ref. 3537. Veith, G.D. and Broderius. Structure-Toxicity Relationships for Industrial Chemicals Causing Type (II) Narcosis Syndrome. In KLE Kaiser (ed.) QSAR in Environmental Toxicology-II, D. Reidel Publ. Co. Dordrecht, Holland:385-391. 1987.
Code	96-hr LC-50		
Species	Fathead Minnow		
Aquatic—Saltwater—Chronic			
AWQC	µg/L		
Code			
Species			
Aquatic—Saltwater—Acute			
AWQC	µg/L		
Code			
Species			

Pollutant: Bromobenzene			CAS: 108861
Variable	Units	Value	Source
Human Health			
q1*	mg/kg-day		Region 3. Risk-based Concentration Table. Oct. 8, 2004. EPA provisional peer-reviewed value.
Carcinogen flag	Y/N	N	
RfD	mg/kg-day	2.00e-2	
Code			
BCF	L/kg	94	ASTER. 2005. Ref. 7. Veith, GD and P Kosian. Estimating Bioconcentration Potential from Octanol/Water Partition Coefficients. In D. Mackay et al. (Eds.) Physical behavior of PCBs in the Great Lakes. Ann Arbor Scie. Publ. Ann Arbor, MI:269-282.
BAF			
RSC			
Aquatic—Freshwater—Chronic			
AWQC	µg/L	560	ASTER. 2005: Ref. 4343. Marchini, S, MD Hoglund, S.J Borderius, and ML Tosato. Comparison of the Susceptibility of Daphnids and Fish to Benzene Derivatives. Sci. Total Environ. Suppl:399-808. 1993.
Code	Estimated From Acute Value Using Acute-Chronic Ratio of 10; See U.S. EPA. Technical Support Document for Water Quality-based Toxics Control. EPA 505/2-90-001. March 1991.		
73Species	Fathead Minnow		
Aquatic—Freshwater—Acute			
AWQC	µg/L	5600	ASTER. 2005: Ref. 4343. Marchini, S, MD Hoglund, S.J Borderius, and ML Tosato. Comparison of the Susceptibility of Daphnids and Fish to Benzene Derivatives. Sci. Total Environ. Suppl:399-808. 1993.
Code	lowest LC ₅₀		
Species	Fathead Minnow		
Aquatic—Saltwater—Chronic			
AWQC	µg/L		Nothing in ASTER.
Code			
Species			
Aquatic—Saltwater—Acute			
AWQC	µg/L		ASTER data cites one reference that used body burden (mmol/kg), and did not pass filter.
Code			
Species			

Pollutant: tributyltin (TBT) (Organotins)			CAS: 668-73-3
Variable	Units	Value	Source
Human Health			
q1*	mg/kg-day		No data (IRIS, USEPA Region RBC Table, ATSDR toxicological profiles, USEPA 2000 [California], USEPA 1995[Great Lakes]).
Carcinogen flag	Y/N		
RfD	mg/kg-day		
Code			
BCF	L/kg	501	Tsuda T, Nakanishi, S. Aoki, and S. Takebayashi. Bio concentration and metabolism of butyltin compounds in carp. Water Res. 22: 647-651. 1988. in EPA. 2003. Ambient Aquatic Life Water Quality Criteria for Tributyltin (TBT)-Final. EPA 822-R-03-031. December.
BAF			
RSC			
Aquatic—Freshwater—Chronic			
AWQC	µg/L	0.072	EPA. 2003. Ambient Aquatic Life Water Quality Criteria for Tributyltin (TBT)-Final. EPA 822-R-03-031. December.
Code	EPA Criteria		
Species	None listed.		
Aquatic—Freshwater—Acute			
AWQC	µg/L	0.46	EPA. 2003. Ambient Aquatic Life Water Quality Criteria for Tributyltin (TBT)-Final. EPA 822-R-03-031. December.
Code	EPA Criteria		
Species	None listed.		
Aquatic—Saltwater—Chronic			
AWQC	µg/L	0.0074	EPA. 2003. Ambient Aquatic Life Water Quality Criteria for Tributyltin (TBT)-Final. EPA 822-R-03-031. December.
Code	EPA Criteria		
Species	None listed.		
Aquatic—Saltwater—Acute			
AWQC	µg/L	0.42	EPA. 2003. Ambient Aquatic Life Water Quality Criteria for Tributyltin (TBT)-Final. EPA 822-R-03-031. December.
Code	EPA Criteria		
Species	None listed.		

Pollutant: Perchlorate			CAS: 14797730
Variable	Units	Value	Source
Human Health			
q1*	mg/kg-day		
Carcinogen flag	Y/N	N	
RfD	mg/kg-day	7.0e-4	IRIS. 2005. 2005 revision. For perchlorate and perchlorate salts.
Code			
BCF	L/kg	1	assumption
BAF			
RSC			
Aquatic—Freshwater—Chronic			
AWQC	µg/L	1.0e5	Data for potassium perchlorate. ASTER. 2005. Ref.: 16030. Youson, JH, JA Holmes, and JF Leatherland. Serum Concentrations of Thyroid Hormones in KClO4-treated Larval Dea Lampreys (Petromyzon marinus K.) Comp. Biochem. Physiol. 111c(2):265-270. 1995.
Code	122-day exposure, hormonal effect		
Species	Sea Lamprey		
Aquatic—Freshwater—Acute			
AWQC	µg/L		Only 100% mortality concentration after 96-hr exposure; cannot adjust to LC50.
Code			
Species			
Aquatic—Saltwater—Chronic			
AWQC	µg/L		No data
Code			
Species			
Aquatic—Saltwater—Acute			
AWQC	µg/L		No data
Code			
Species			

Pollutant: RDX			CAS: 121824
Variable	Units	Value	Source
Human Health			
q1*	mg/kg-day	1.1e-1	IRIS. 2005. 1993 revision. C: possible human carcinogen.
Carcinogen flag	Y/N	Y	
RfD	mg/kg-day	3.0e-3	IRIS. 2005. 1993 revision.
Code			
BCF	L/kg		
BAF			
RSC			
Aquatic—Freshwater—Chronic			
AWQC	µg/L	1350	ASTER, 2005. Ref: 17503.Burton, D.T., S.D. Turley, and G.T. Peters. The Acute and Chronic Toxicity of Hexahydro-1,3,5-Trinitro-1,3,5-Triazine (RDX) to the Fathead Minnow (Pimephales promelas). Chemosphere 29(3):567-579. 1994 B
Code	32-day NOEC		
Species	Fathead Minnow		
Aquatic—Freshwater—Acute			
AWQC	µg/L	12700	ASTER, 2005. Ref: 17503.Burton,D.T., S.D. Turley, and G.T. Peters. The Acute and Chronic Toxicity of Hexahydro-1,3,5-Trinitro-1,3,5-Triazine (RDX) to the Fathead Minnow (Pimephales promelas). Chemosphere 29(3):567-579. 1994 B
Code	96-hr LC ₅₀		
Species	Fathead Minnow		
Aquatic—Saltwater—Chronic			
AWQC	µg/L		no data
Code			
Species			
Aquatic—Saltwater—Acute			
AWQC	µg/L		no data
Code			
Species			

Pollutant: atrazine-desethyl			CAS: 6190654
Variable	Units	Value	Source
Human Health			
q1*	mg/kg-day		No data (IRIS, USEPA Region RBC Table, ATSDR toxicological profiles, USEPA 2000 [California], USEPA 1995[Great Lakes]).
Carcinogen flag	Y/N		
RfD	mg/kg-day		
Code			
BCF	L/kg		
BAF			
RSC			
Aquatic—Freshwater—Chronic			
AWQC	µg/L		no ASTER data.
Code			
Species			
Aquatic—Freshwater—Acute			
AWQC	µg/L		no ASTER data.
Code			
Species			
Aquatic—Saltwater—Chronic			
AWQC	µg/L		no ASTER data.
Code			
Species			
Aquatic—Saltwater—Acute			
AWQC	µg/L		no ASTER data.
Code			
Species			

Pollutant: Triazines			CAS:
Variable	Units	Value	Source
Human Health			
q1*	mg/kg-day	1.3e-1	Geometric mean of values for atrazine, cyanazine, and simazine. IRIS. 2005.
Carcinogen flag	Y/N	Y	
RfD	mg/kg-day	7.0e-3	Geometric mean of values for atrazine, cyanazine, and simazine. Region 3. Risk Based Concentration Table. 2004. HEAST
Code			
BCF	L/kg	13	Geometric mean of values for atrazine, cyanazine, and simazine.
BAF			
RSC			
Aquatic—Freshwater—Chronic			
AWQC	µg/L	61	Geometric mean of values for atrazine, cyanazine, and simazine.
Code			
Species			
Aquatic—Freshwater—Acute			
AWQC	µg/L	29,000	Geometric mean of values for atrazine and simazine.
Code			
Species			
Aquatic—Saltwater—Chronic			
AWQC	µg/L		.
Code			
Species			
Aquatic—Saltwater—Acute			
AWQC	µg/L	2,600	Value for atrazine.
Code			
Species			

Pollutant: Atrazine			CAS: 1912249
Variable	Units	Value	Source
Human Health			
q1*	mg/kg-day	2.2e-1	IRIS. 2005.
Carcinogen flag	Y/N	Y	
RfD	mg/kg-day	2.5e-2	Region 3. Risk Based Concentration Table. 2004. HEAST
Code			
BCF	L/kg	31	ASTER. 2005. Ref. 7. Veith, GD and P Kosian. Estimating Bioconcentration Potential from Octanol/Water Partition Coefficients. In D. Mackay et al. (Eds.) Physical behavior of PCBs in the Great Lakes. Ann Arbor Scie. Publ. Ann Arbor, MI:269-282.
BAF			
RSC			
Aquatic—Freshwater—Chronic			
AWQC	µg/L	65	ASTER. 2005. Ref. 631. Macek, KJ KS Buxton, S Sauter, S Gnilka, and JW Dean. Chronic Toxicity of Atrazine to Selected Aquatic Invertebrates and Fishes. Ecol. Res. Serv. EPA 600/3-76-047. Environ. Res. Lab., U.S., EPA, Duluth:MN 50 pp. 1976.
Code	mortality		
Species	Brook Trout		
Aquatic—Freshwater—Acute			
AWQC	µg/L	6,700	ASTER. 2005. Ref. 17138. Brooke. LT. Results of Freshwater Exposures with the Chemicals Atrazine, Biphenyl, Carbaryl, Carbazole, Dibenzofuran, 3,3-dichorobenzidine... Center for Lake Superior Environmental Studies, University of Wisconsin, 1991.
Code	96-hr LC ₅₀		
Species	Stone Fly		
Aquatic—Saltwater—Chronic			
AWQC	µg/L		.
Code			
Species			
Aquatic—Saltwater—Acute			
AWQC	µg/L	2,600	ASTER. 2005. Ref. 14715. Hall, LW Jr., MC Zeigenfuss, RD Anderson, TD Spittler, and HC Leichtweis. Influence of Salinity on Atrazine Toxicity to a Chesapeake Bay Copepod (Eurytemora affinis) and Fish (Cyprindon variegatus). Estuaries 17(1B):181-186. 1994.
Code	96-hr LC ₅₀		
Species	Calanoid copepod		

Pollutant: Simazine			CAS: 122349
Variable	Units	Value	Source
Human Health			
q1*	mg/kg-day	1.2e-1	Region 3. Risk Based Concentration Table. 2004. HEAST
Carcinogen flag	Y/N	Y	
RfD	mg/kg-day	5.00e-3	IRIS. 2005. 1994 revision.
Code			
BCF	L/kg	18	ASTER, 2005. Ref. 7. Veith, GD and P Kosian. Estimating Bioconcentration Potential from Octanol/Water Partition Coefficients. In D. Mackay et al. (Eds.) Physical behavior of PCBs in the Great Lakes. Ann Arbor Scie. Publ. Ann Arbor, MI:269-282.
BAF			
RSC			
Aquatic—Freshwater—Chronic			
AWQC	µg/L	1000	ASTER. 2005. Ref. 10969. McGinty, AS. Effects of Periodic Applications of Simazine on the Production of Tilapia nilotica Fingerlings. J. Agric. Univ. P.R. 68(4):467-469. 1984.
Code	mortality		
Species	Nile Tilapia		
Aquatic—Freshwater—Acute			
AWQC	µg/L	124,875	ASTER. 2005. Ref. 15823. Veith GD, DJ Call, and LT Brooke. Structure-Toxicity Relationships for the Fathead Minnow, Pimephales promelas: Narcotic Industrial Chemicals. Can. J. Fish. Aquat. Scie. 40(6):743-748. 1983.
Code	96-hr LC ₅₀		
Species	Fathead Minnow		
Aquatic—Saltwater—Chronic			
AWQC	µg/L		.
Code			
Species			
Aquatic—Saltwater—Acute			
AWQC	µg/L		
Code			
Species			

Pollutant: Cyanazine			CAS: 2125462
Variable	Units	Value	Source
Human Health			
q1*	mg/kg-day	8.4e-1	Region 3. Risk Based Concentration Table. 2004. HEAST
Carcinogen flag	Y/N	Y	
RfD	mg/kg-day	2.0e-3	Region 3. Risk Based Concentration Table. 2004. HEAST
Code			
BCF	L/kg	4	ASTER, 2005. Ref. 7. Veith, GD and P Kosian. Estimating Bioconcentration Potential from Octanol/Water Partition Coefficients. In D. Mackay et al. (Eds.) Physical behavior of PCBs in the Great Lakes. Ann Arbor Scie. Publ. Ann Arbor, MI:269-282.
BAF			
RSC			
Aquatic—Freshwater—Chronic			
AWQC	µg/L	3.5	ASTER. 2005. Ref. 4442. Davies, PE, LSJ Cook, and D Goenarso. Sublethal Responses to Pesticides of Several Species of Australian Freshwater Fish and Crustaceans and Rainbow Trout. Environ. Toxicol. Chem. 13(8):1341-1354. 1994.
Code	10-day LC ₅₀		
Species	Rainbow Trout		
Aquatic—Freshwater—Acute			
AWQC	µg/L		
Code			
Species			
Aquatic—Saltwater—Chronic			
AWQC	µg/L		.
Code			
Species			
Aquatic—Saltwater—Acute			
AWQC	µg/L		
Code			
Species			

Pollutant: DCPA mono-acid degradate			CAS: 887547
Variable	Units	Value	Source
Human Health			
q1*	mg/kg-day		No data (IRIS, USEPA Region RBC Table, ATSDR toxicological profiles, USEPA 2000 [California], USEPA 1995[Great Lakes]).
Carcinogen flag	Y/N		
RfD	mg/kg-day		
Code			
BCF	L/kg		
BAF			
RSC			
Aquatic—Freshwater—Chronic			
AWQC	µg/L		no ASTER data.
Code			
Species			
Aquatic—Freshwater—Acute			
AWQC	µg/L		no ASTER data.
Code			
Species			
Aquatic—Saltwater—Chronic			
AWQC	µg/L		no ASTER data.
Code			
Species			
Aquatic—Saltwater—Acute			
AWQC	µg/L		no ASTER data.
Code			
Species			

Pollutant: DCPA di-acid degradate			CAS: 2136790
Variable	Units	Value	Source
Human Health			
q1*	mg/kg-day		No data (IRIS, USEPA Region RBC Table, ATSDR toxicological profiles, USEPA 2000 [California], USEPA 1995[Great Lakes]).
Carcinogen flag	Y/N		
RfD	mg/kg-day		
Code			
BCF	L/kg	179	ASTER, 2005. Ref. 7. Veith, GD and P Kosian. Estimating Bioconcentration Potential from Octanol/Water Partition Coefficients. In D. Mackay et al. (Eds.) Physical behavior of PCBs in the Great Lakes. Ann Arbor Scie. Publ. Ann Arbor, MI:269-282.
BAF			
RSC			
Aquatic—Freshwater—Chronic			
AWQC	µg/L	1364	ASTER, 2005. Ref: 15823. Veith GD, DJ Call, and LT Brooke. Structure-Toxicity Relationships for the Fathead Minnow, Pimephales promelas: Narcotic Industrial Chemicals. Can. J. Fish. Aquat. Scie. 40(6):743-748. 1983.
Code	Estimated From Acute Value Using Acute-Chronic Ratio of 10; See U.S. EPA. Technical Support Document for Water Quality-based Toxics Control. EPA 505/2-90-001. March 1991.		
Species	Fathead Minnow		
Aquatic—Freshwater—Acute			
AWQC	µg/L	13644	ASTER, 2005. Ref: 15823. Veith GD, DJ Call, and LT Brooke. Structure-Toxicity Relationships for the Fathead Minnow, Pimephales promelas: Narcotic Industrial Chemicals. Can. J. Fish. Aquat. Scie. 40(6):743-748. 1983.
Code	96-hr LC ₅₀		
Species	Fathead Minnow		
Aquatic—Saltwater—Chronic			
AWQC	µg/L		no ASTER data.
Code			
Species			
Aquatic—Saltwater—Acute			
AWQC	µg/L		no ASTER data.
Code			
Species			

Pollutant: Nicotine			CAS: 54115
Variable	Units	Value	Source
Human Health			
q1*	mg/kg-day		none identified
Carcinogen flag	Y/N		
RfD	mg/kg-day		none identified
Code			
BCF	L/kg	4	ASTER, 2005. Ref. 7. Veith, G.D. and Kosian. Estimating Bioconcentration Potential from Octanol/Water Partition Coefficients. In D. Mackay et. al. (Eds.), Physical Behavior of PCBs in the Great Lakes. Ann Arbor Sci. Publ., Ann Arbor, MI:269-282. 1983. (QSAR.)
BAF			
RSC			
Aquatic—Freshwater—Chronic			
AWQC	µg/L	3490	ASTER, 2005. Ref. 16362. Passino-Reader, DR, WH Berlin, and JP Hickey. Chronic Bioassays of Rainbow Trout Fry with Compounds Representative of Contaminants in Great Lakes Fish. J. Great Lakes Res. 21(3):373-383. 1995. Geometric average of LOEC=4200 and NOEC=2900.
Code	MATC		
Species	Rainbow Trout		
Aquatic—Freshwater—Acute			
AWQC	µg/L		
Code			
Species			
Aquatic—Saltwater—Chronic			
AWQC	µg/L		
Code			
Species			
Aquatic—Saltwater—Acute			
AWQC	µg/L		
Code			
Species			